

MOLECULAR SPECTRA *and* MOLECULAR STRUCTURE

IV. CONSTANTS OF DIATOMIC MOLECULES

By

K. P. Huber and G. Herzberg

National Research Council of Canada



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PREFACE

Since the publication in 1950 of Vol. I, *Spectra of Diatomic Molecules of Molecular Spectra and Molecular Structure*, much progress has been made in the field. While there have been some important refinements in the theory of diatomic molecular spectra, most of the advances have been in the further exploration of individual spectra. Not only has the number of molecules about which some spectroscopic data are available been increased by a factor of 2 to 3, but also the spectroscopic information about the molecules known in 1950 has been vastly extended. This is due to the observation of new electronic states (about three times as many as known before), the enormous improvements in the accuracy of the constants of the states known in 1950, and the determination of higher order constants.

In view of the increasing use of spectroscopic information on diatomic molecules in other fields of physics, in chemistry, and in astrophysics, it appeared desirable to prepare an up-to-date version of the table of molecular constants in the appendix of Vol. I. This updating proved to be far more time-consuming than originally anticipated, and it is only now, 10 years after its initiation, that we are able to present such a table, which, instead of the original 80 pages (plus 30 pages of bibliography), now fills a volume of 700 pages.

In the interest of economy, and unlike the original version, the new table has been produced by photo-offset from the final manuscript. Thus, typographical errors, which would have been likely to occur in such a difficult typesetting job, were entirely eliminated. We have spared no effort to make the table as up-to-date as possible. The date of final revision of each part is indicated. While the principal constants of each state of each molecule are listed uniformly in the body of the table, additional constants that could not be fitted in are given in the footnotes. Also, many qualifications and other explanations are added in this way.

We hope that users of these tables will find them helpful in supplying up-to-date constants as well as references to the most recent literature.

We are greatly indebted to many colleagues who have supplied advance

information on recent unpublished work. The tables edited by the late B. Rosen were of great help to us in finding some of the earlier literature on many of the molecules dealt with therein. We have also greatly profited by the special tables prepared by P. H. Krupenie on O_2 and CO and by Krupenie and A. Lofthus on N_2 . But wherever possible we have checked with the original publications. Particularly valuable to us throughout the entire course of this work were the *Berkeley Newsletters* prepared by J. G. Phillips and S. P. Davis; without them, a great many of the publications listed in the tables and in the appendix might have escaped our attention.

Although the final manuscript was prepared by one of us (K.P.H.), many drafts of the tables were typed by M. P. Thompson, and much checking of numbers and references was done by her and I. Dabrowski. We are most grateful for their efforts.

Finally, we must acknowledge that the National Research Council of Canada supported this work throughout the protracted period of its preparation by permitting one of us to spend all of his time for more than 10 years—and the other, part of his time—on this project and by providing other necessary facilities.

Ottawa (Canada), May 1978

K. P. HUBER
G. HERZBERG

INTRODUCTION

In this volume, we present a compilation of available data for all diatomic molecules and ions. The format of most of the tables follows closely that used in Table 39 of Volume I¹ of this series; that is, the various known electronic states and their symmetry symbols appear in the first column, and in the adjacent columns the electronic energy (T_e), the vibrational constants (ω_e and $\omega_e x_e$), the rotational constants (B_e , α_e , D_e), and the internuclear distance (r_e) are given. In the last three columns, the observed transitions involving the particular electronic state, their ν_{00} values, and the references on which the information is based are listed. The columns " $\omega_e y_e$ " and "Remarks" of the previous table have been omitted, but this information is given in the footnotes. In addition, in the footnotes, references about Franck-Condon factors, potential functions, and other constants are given such as the following:

- A Spin-orbit interaction parameter
- λ Spin-spin interaction parameter
- γ Spin-rotation interaction parameter (not to be confused with the rotation-vibration interaction constant, γ_e)
- τ Radiative lifetime
- f Oscillator strength (f value)
- μ_{el} Electric dipole moment in Debye units (1 D = 10^{-18} esu cm).
- g_J Rotational g factor in units of nuclear magnetons (μ_N)
- Λ -type doubling constants p , q , . . .
- Hyperfine structure (hfs) constants such as the magnetic coupling constants, a , b , c , d , and the electric quadruple coupling constant, eqQ .

At the top of each table, the reduced mass μ of the molecule is given, as well as the dissociation energy D_0^0 in the ground state and the ionization potential (I.P.). Dissociation energies for states other than the ground state are easily derived if the dissociation products are known. Normally they are not listed explicitly.

¹G. Herzberg, *Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules*, 2nd ed., Van Nostrand (1950).

The data presented in the tables come from a wide variety of experimental and theoretical studies. Of these, the most important are electronic spectra in emission or absorption (extending from the infrared to the vacuum ultraviolet and, in a few cases, the X-ray region), rotation-vibration spectra in the near infrared, rotation spectra in the far infrared and especially in the microwave (centimeter, millimeter, and submillimeter wave) regions. Additional highly precise information comes for some molecules from molecular beam electric and magnetic resonance studies and electron spin resonance spectra. Still other information has been taken from photofragment spectra, photoelectron and photoion spectra, and Auger electron spectra. In addition, data from electron scattering (elastic and inelastic), atomic scattering, mass spectrometry, flame photometry, and thermochemical studies have been used. References to lifetime measurements by various methods are also included, as well as references to theoretical calculations, which may be compared with experimental data or may fill gaps in existing experimental information.

The molecules are listed in strict alphabetical order (e.g., BaBr, BaCl precede BBr and BCl, even though this separates the latter from B₂). Positive and negative ions, in this order, follow immediately after the corresponding neutral molecule. Constants for hydrides, deuterides, and tritiides are given separately; for all other molecules, they are given for only one, usually the most abundant, isotope or for the natural isotopic mixture. In the latter case, the mass number for the most abundant species of one or both of the constituent atoms appears in parentheses and the reduced mass μ , also in parentheses, has been calculated accordingly.²

As in Volume I, the footnotes are referred to by lower-case letters^{a,b,c,...} continuing where necessary with ^{a',b',c',...}. In tables that extend over several pages, the sequence of footnotes starts with ^a on each page.

The references to the original literature are numbered in chronological order for each molecule and follow immediately at the end of the corresponding table. In order to save space, they are given in abbreviated form, omitting the initials of the authors and using code names for the journals as well as for the monographs. An alphabetical list of these abbreviated publication titles may be found on pages 1 through 7.

Each table carries the date (month and year) of its last revision. Considering the inevitable delay between publication of a paper and its eventual digestion for the purpose of the table, we estimate that the information in the table can be regarded as complete up to an effective cutoff time of three or four months prior to the indicated date. When the date is followed by the letter A, it indicates that in the appendix on pages 690 through 716 a list and short description may be found of additional publications that came to our notice after completion of the particular table.

²For ions with unequal nuclear charges, the reduced mass is not given explicitly. An ambiguity arises here with respect to the calculation of μ , which we did not undertake to resolve; instead, we used the reduced mass of the corresponding neutral molecule for the evaluation of internuclear distances. This approximation will normally not significantly increase the uncertainty of the result.

The notation for spectra of diatomic molecules has been standardized for many years. We have followed this notation throughout this volume. There is one important change in the notation, which was internationally agreed upon after the publication of Volume I: the change from K to N for the angular momentum excluding electron spin and the corresponding quantum number. There are still authors who are not aware of this change, which was agreed upon because, in polyatomic molecules, K represents the component of J in the direction of the top axis, and both K and N are needed there when $S \neq 0$.

All numbers in the tables are in cm^{-1} units except where otherwise indicated. The conversion factors and fundamental constants which we have used are based on "The 1973 Least-Squares Adjustment of the Fundamental Constants" by Cohen and Taylor (*J. Phys. Chem. Ref. Data* 2 [4], 663-734 [1973]). The most important of these are the following:

$$\begin{aligned}
 1 \text{ eV} &= 8065.47_9 \text{ cm}^{-1} \\
 1 \text{ kcal/mol} &= 349.75_5 \text{ cm}^{-1} \\
 1 \text{ kJ/mol} &= 83.5935 \text{ cm}^{-1} \\
 c &= 2.99792458 \times 10^{10} \text{ cm s}^{-1} \\
 \frac{m(^{12}\text{C})}{12} &= 1.6605655 \times 10^{-24} \text{ g} \\
 \frac{h}{8\pi^2 c} &= 27.9932_0 \times 10^{-40} \text{ g cm}^2 \text{ cm}^{-1} \\
 &= 16.8576_3 \text{ a.m.u. } \text{\AA}^2 \text{ cm}^{-1} \\
 \frac{k}{hc} &= 0.695030 \text{ K}^{-1} \text{ cm}^{-1} \\
 1 \text{ K} &= 0.000086173 \text{ eV}
 \end{aligned}$$

The reduced masses are referred to $m(^{12}\text{C}) = 12.00000000$ and are calculated from the atomic masses given in the table by Wapstra and Gove (*Nucl. Data Tables* 9, 265-301 [1971]).

All the data in the table have been reviewed critically. They are, however, presented without error limits. The addition of meaningful and uniformly evaluated error limits would have meant an enormous increase in the time required to complete these tables. Instead, we hope that the number of digits quoted may serve as a *very* rough indication of the estimated order of magnitude of the error, generally ± 9 units of the last decimal place. Where the last digit is given as a subscript, we expect that the uncertainty may considerably exceed ± 10 units of that last decimal place.

In almost all cases, and unless stated otherwise, the constants ω_e , $\omega_e x_e$, B_e , α_e , and D_e that are listed are effective constants; that is, apart from sign they correspond to the coefficients Y_{lm} in the Dunham series expansion for the term values

$$T_{vJ} = \sum_{lm} Y_{lm} (v + \frac{1}{2})^l J^m (J + 1)^m$$

The signs are defined as follows:

$$\begin{aligned}
 G(v) &= \omega_e(v + \tfrac{1}{2}) - \omega_e x_e(v + \tfrac{1}{2})^2 + \omega_e y_e(v + \tfrac{1}{2})^3 \\
 &\quad + \omega_e z_e(v + \tfrac{1}{2})^4 + \dots \\
 F_v(J) &= B_v J(J + 1) - D_v J^2(J + 1)^2 + H_v J^3(J + 1)^3 \dots \\
 B_v &= B_e - \alpha_e(v + \tfrac{1}{2}) + \gamma_e(v + \tfrac{1}{2})^2 + \dots \\
 D_v &= D_e + \beta_e(v + \tfrac{1}{2}) + \dots
 \end{aligned}$$

The higher order constants are given in the footnotes.

T_e is usually calculated from the observed transitions without taking into account the quantity Y_{00} in the upper or lower state. Exceptions are mentioned in the footnotes.

The dissociation energy D_0^0 is always defined as *the energy of the ground state atomic products relative to the lowest existing level of the molecule*. In almost all cases, there is a footnote after D_0^0 , which explains the method used in its derivation. The description "thermochemical value" is used to indicate any determination (mass spectrometric, flame photometric, or other) that involves the evaluation of a thermochemical equilibrium. Where necessary, thermochemical values that have been derived from exchange reactions have been adjusted to take account of recent changes in the dissociation energies of the reference molecules.

In agreement with common practice, the first ionization potential (in eV) is taken as *the energy difference of the lowest existing level of the ion and the lowest existing level of the neutral system*. Analogous definitions apply to positive as well as negative ions although, for the latter, the I.P. is more commonly referred to as electron affinity of the neutral. Higher ionization potentials have in some cases been added in the table or in the footnotes. Electron impact appearance potentials have only rarely been included since their accuracy is usually low (typically ± 0.5 eV).

It appears nearly impossible to give a generally applicable definition of the band origins. Here, origins in singlet systems normally refer to the zero lines; that is, they include the J independent term $-B\Lambda^2$, which some authors prefer to include in the rotational energy expression. Similarly, for case "a" multiplet states, a corresponding definition applies to individual sub-bands; exceptions to these rules are usually indicated in the footnotes. For intermediate coupling or coupling close to case "b", we frequently refer to the zero-point of the Hill-Van Vleck (or equivalent) expression; an explanation is usually given in the footnotes. Multiplets very close to case "b" are often treated as singlets disregarding electron spin. In all cases where our definition of the origin deviates strongly from that used by the original author, we have indicated this in the accompanying footnote.

The magnitude and sign of the Λ -type doubling is indicated in many instances in footnotes by quoting either the difference $B(R, P) - B(Q)$, which is equivalent to $B(\Pi^+) - B(\Pi^-)$ for transitions involving a Σ^+ state, or the leading terms in the expression giving the observed splitting as a function of J . For

the labeling of the parity doublet levels, we have adopted the recommendations of Brown et al. (*J. Mol. Spectrosc.* **55**, 500 [1975]):

integral J : e levels have parity $+(-1)^J$
 f levels have parity $-(-1)^J$
 half-integral J : e levels have parity $+(-1)^{J-\frac{1}{2}}$
 f levels have parity $-(-1)^{J-\frac{1}{2}}$

The sign of the splitting is defined by

$$\Delta\nu_{ef}(J) = F_e(J) - F_f(J) = -\Delta\nu_{fe}(J)$$

For some case “ b ” $^2\Pi$ states we give $\Delta\nu_{ef}(N)$ and refer to the F_1 component.

The following symbols are used throughout the table:

- H Data obtained from band head measurements
 - Z Data obtained from, or referring to, band origins
 - R Shaded towards longer wavelengths
 - V Shaded towards shorter wavelengths
 - () Uncertain data
 - [] Data refer to $v = 0$ or lowest observed level. T_e values in square brackets give the energy of this level relative to the minimum of the ground-state potential energy curve. Vibrational frequencies in square brackets correspond to $\Delta G(\frac{1}{2})$ or the lowest observed integral.
 - { } Hypothetical levels
 - Emission
 - ← Absorption
 - ↔ Emission and absorption
 - * Indicates a reference number where a good record or reproduction of the spectrum may be found
- $\left. \begin{array}{l} \text{According to international agreement the} \\ \text{upper state always comes first.} \end{array} \right\}$

CONTENTS

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MOLECULAR SPECTRA
and
MOLECULAR STRUCTURE

IV. CONSTANTS OF DIATOMIC
MOLECULES

ABBREVIATED PUBLICATION TITLES.

AA	Astronomy and Astrophysics.
AA(Suppl.)	Astronomy and Astrophysics, Supplement Series.
AANL	Atti della (Reale) Accademia Nazionale dei Lincei. Rendiconti, Classe di Scienze Fisiche, Matematiche e Naturali.
AAp	Annales d'Astrophysique.
AAQA	Anales de la Asociacion Quimica Argentina.
AC(Int. Ed. Engl.)	Angewandte Chemie. International Edition in English.
AD	Atomic Data.
AdC	Advances in Chemistry Series.
AdGp	Advances in Geophysics.
AdHTC	Advances in High Temperature Chemistry.
ADNDT	Atomic Data and Nuclear Data Tables.
AdRS	Advances in Raman Spectroscopy.
AF	Arkiv foer Fysik.
AGEP	Annales de Géophysique.
AMAF	Arkiv foer Matematik, Astronomi och Fysik.
AO	Applied Optics.
AP(Leipzig)	Annalen der Physik (Leipzig).
AP(Paris)	Annales de Physique (Paris).
APH	Acta Physica Academiae Scientiarum Hungaricae.
ApJ	Astrophysical Journal.
ApJ(Suppl.)	Astrophysical Journal, Supplement Series.
APL	Applied Physics Letters.
ApL	Astrophysical Letters.
APP	Acta Physica Polonica.
ARAA	Annual Review of Astronomy and Astrophysics.
ARSEFQ	Anales de la Real Sociedad Espanola de Fisica y Quimica.
AS	Applied Spectroscopy.
AZ	Astronomicheskii Zhurnal. - For English translation see SAAJ.

BAMS	Berkeley Analyses of Molecular Spectra. University of California Press. <u>1</u> S. P. Davis, J. G. Phillips, "The Red System ($A^2\Pi-X^2\Sigma$) of the CN Molecule" (1963). <u>2</u> J. G. Phillips, S. P. Davis, "The Swan System of the C_2 Molecule"; "The Spectrum of the HgH Molecule" (1968).
BAPS	Bulletin of the American Physical Society.
BAPS(MAP)	Bulletin de l'Académie Polonaise des Sciences. Série des Sciences Mathématiques, Astronomiques et Physiques.
BASPS	Bulletin of the Academy of Sciences of the USSR, Physical Series. - English translation of IANSF.
BBPC	Berichte der Bunsen-Gesellschaft für Physikalische Chemie.
BCSARB	Bulletin de la Classe des Sciences, Académie Royale de Belgique.
BSCB	Bulletin des Sociétés Chimiques Belges.
BSCF	Bulletin de la Société Chimique de France.
BSRSL	Bulletin de la Société Royale des Sciences de Liège.
CaP	Cahiers de Physique.
CC	Chemical Communications.
CCA	Croatica Chemica Acta.
CF	Combustion and Flame.
CJC	Canadian Journal of Chemistry.
CJP	Canadian Journal of Physics.
CJPS	Chinese Journal of Physics. (Chinese Physical Society) Shanghai.
CJR	Canadian Journal of Research.
CJS	Canadian Journal of Spectroscopy.
CP	Chemical Physics.
CPAS	Commentarii, Pontificia Academia Scientiarum.
CPL	Chemical Physics Letters.
CR	Comptes Rendus Hebdomadaires des Seances de l'Académie des Sciences. Paris.
CRev	Chemical Reviews.
CS	Current Science.
CSp	Canadian Spectroscopy.
DANS	Doklady Akademii Nauk SSSR. - For English translation see DC, DPC.
DC	Doklady Chemistry. - English translation of DANS (Chemistry Section).
DFS	Discussions of the Faraday Society.
DISSEN	A. G. Gaydon, "Dissociation Energies and Spectra of Diatomic Molecules", 3rd ed., Chapman and Hall (1968).
DONNSPEC	Tables Internationales de Constantes Sélectionnées. 17. Données Spectroscopiques relatives aux Molécules Diatomiques (établi sous la direction de B. Rosen). Pergamon Press (1970).

DPC	Doklady Physical Chemistry. - English translation of DANS (Physical Chemistry Section).
FDSCS	Faraday Discussions of the Chemical Society.
Fizika	Fizika (Zagreb).
FSCS	Faraday Symposia of the Chemical Society.
GCI	Gazzetta Chimica Italiana.
GHDB	Glasnik Hemijskog Drustva, Beograd. (Bulletin of the Chemical Society, Belgrade.)
HCA	Helvetica Chimica Acta.
HPA	Helvetica Physica Acta.
HT(USSR)	High Temperature. - English translation of TVT.
HTS	High Temperature Science.
IAMS	Identification Atlas of Molecular Spectra. U. of Western Ontario (1964/5), York University (1967/72). <ol style="list-style-type: none"> <u>1</u> D.C. Tyte, R.W. Nicholls, "The $\text{AlO } A^2\Sigma-X^2\Sigma$ Blue-Green System" (1964). <u>2</u> D.C. Tyte, R.W. Nicholls, "The $\text{N}_2 \text{ C}^3\Pi_u-B^3\Pi_g$ Second Positive System" (1964). <u>3</u> D.C. Tyte, R.W. Nicholls, "The $\text{N}_2^+ B^2\Sigma_u^+-X^2\Sigma_g^+$ First Negative System of Nitrogen" (1965). <u>4</u> G.R. Hébert, S.H. Innanen, R.W. Nicholls, "The $\text{O}_2 B^3\Sigma_u^--X^3\Sigma_g^-$ Schumann-Runge System" (1967). <u>5</u> D.C. Tyte, S.H. Innanen, R.W. Nicholls, "The $\text{C}_2 A^3\Pi_g-X'^3\Pi_u$ Swan System" (1967). <u>6</u> V. Degen, S.H. Innanen, G.R. Hébert, R.W. Nicholls, "The $\text{O}_2 A^3\Sigma_u^+-X^3\Sigma_g^-$ Herzberg I System" (1968). <u>7</u> J.A. Harrington, R.M. Seel, G.R. Hébert, R.W. Nicholls, "The $\text{VO C}^4\Sigma^--X^4\Sigma^-$ Yellow-Green and $B^4\Pi-X^4\Sigma^-$ Red Systems" (1970). <u>8</u> B. Brocklehurst, G.R. Hébert, S.H. Innanen, R.M. Seel, R.W. Nicholls, "The $\text{CN } A^2\Pi-X^2\Sigma^+$ Red System" (1971). <u>9</u> B. Brocklehurst, G.R. Hébert, S.H. Innanen, R.M. Seel, R.W. Nicholls, "The $\text{CN } B^2\Sigma^+-X^2\Sigma^+$ Violet System" (1972).
IANNM	Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy. - For English translation see IM.
IANSF	Izvestiya Akademii Nauk SSSR, Seriya Fizicheskaya. - For English translation see BASPS.
Icarus	Icarus.
ICB	Industrie Chimique Belge.
IDSPEC	R.W. B. Pearse, A.G. Gaydon, "The Identification of Molecular Spectra". Chapman and Hall, 3rd ed. 1963, 4th ed. 1976.
IJMSIP	International Journal of Mass Spectrometry and Ion Physics.
IJP	Indian Journal of Physics.
IJPAP	Indian Journal of Pure and Applied Physics.
IJQC	International Journal of Quantum Chemistry.
IM	Inorganic Materials. - English translation of IANNM.

INCL	Inorganic and Nuclear Chemistry Letters.
IPCR	See Sci. Pap. IPCR (Tokyo).
ISOANK	Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR, Seriya Khimicheskikh Nauk. - For English translation
IVUZF	Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika. - For English translation see SPJ. see SCJ.
IVUZK	Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya.
JACS	Journal of the American Chemical Society.
JANAF	JANAF Thermochemical Tables. 2nd edition. NSRDS-NBS 37 (1971).
JAP	Journal of Applied Physics.
JAS	Journal of Applied Spectroscopy. - English translation of ZPS.
JATP	Journal of Atmospheric and Terrestrial Physics.
JCP	Journal of Chemical Physics.
JCPPB	Journal de Chimie Physique et de Physico-Chimie Biologique. Paris.
JCS	Journal of the Chemical Society.
JCS FT	Journal of the Chemical Society. Faraday Transactions.
JESRP	Journal of Electron Spectroscopy and Related Phenomena.
JGR	Journal of Geophysical Research.
JIC(USSR)	Journal of Inorganic Chemistry (USSR). - English translation of ZNK.
JINC	Journal of Inorganic and Nuclear Chemistry.
JJP	Japanese Journal of Physics.
JLTP	Journal of Low Temperature Physics.
JMS	Journal of Molecular Spectroscopy.
JMS ^t	Journal of Molecular Structure.
JOSA	Journal of the Optical Society of America.
JP	Journal of Physics.
JP(Paris)	Journal de Physique (Paris), and Journal de Physique (Paris), Lettres.
JPC	Journal of Physical Chemistry.
JPCRD	Journal of Physical and Chemical Reference Data.
JPhoC	Journal of Photochemistry.
JPR	Journal de Physique et le Radium.
JPSJ	Journal of the Physical Society of Japan.
JPUSSR	Journal of Physics (Moscow).
JQE	IEEE Journal of Quantum Electronics.
JQSRT	Journal of Quantitative Spectroscopy and Radiative Transfer.

JRCNRS	Journal des Recherches du Centre National de la Recherche Scientifique.
JRNBS	Journal of Research of the National Bureau of Standards.
JRS	Journal of Raman Spectroscopy.
JSHU	Journal of Science of the Hiroshima University.
JSIR	Journal of Scientific and Industrial Research.
JSRBHU	Journal of Scientific Research of the Banaras Hindu University.
KEM	Kvantovaya Elektronika (Moscow). - For English translation see SJQE.
LNC	Lettere al Nuovo Cimento (della Società Italiana di Fisica).
LTS	Low Temperature Science, Series A: Physical Sciences. (Teion Kagaku, Butsuri-Hen.)
METOX	A. Gatterer, J. Junkes, E. W. Salpeter, B. Rosen, "Molecular Spectra of Metallic Oxides", Specola Vaticana
MOLSPEC	G. Herzberg, "Molecular Spectra and Molecular Structure". Van Nostrand Reinhold. (1957).
	<u>1</u> Spectra of Diatomic Molecules. 2nd ed. (1950).
	<u>2</u> Infrared and Raman Spectra of Polyatomic Molecules (1945).
	<u>3</u> Electronic Spectra and Electronic Structure of Polyatomic Molecules (1966).
MP	Molecular Physics.
MSRSL	Mémoires de la Société Royale des Sciences de Liège (Collection en 8°).
MSRSL*	Mémoires de la Société Royale des Sciences de Liège, Volume hors série.
MUCB	Moscow University Chemistry Bulletin. - English translation of VMUK.
NARSSU	Nova Acta Regiae Societatis Scientiarum Upsaliensis.
Nature	Nature (London).
Nature PS	Nature (London), Physical Sciences.
Naturw.	Naturwissenschaften.
NBSM	National Bureau of Standards (U.S.), Monograph.
NC	Nuovo Cimento (della Società Italiana di Fisica).
NC(Suppl.)	Nuovo Cimento, Supplemento.
NDVSK	Nauchnye Doklady Vysshei Shkoly, Khimiya i Khimicheskaya Tekhnologiya.
NIM	Nuclear Instruments and Methods.
NSRDS-NBS	National Standard Reference Data Series, National Bureau of Standards (U.S.).
OC	Optics Communications.
OPA	Optica Pura y Aplicada.
OS	Optika i Spektroskopiya. - For English translation see OS(Engl. Transl.).
OS(Engl. Transl.)	Optics and Spectroscopy (USSR). - English translation of OS.
PASP	Publications of the Astronomical Society of the Pacific.

PBCS	Proceedings of the British Ceramic Society.
PC	Physics in Canada.
PCS	Proceedings of the Chemical Society, London.
PDAO	Publications of the Dominion Astrophysical Observatory, Victoria, British Columbia.
Physica	Physica.
PIAS	Proceedings of the Indian Academy of Sciences.
PKNaw	Proceedings of the Koninklijke Nederlandse Akademie van Wetenschappen, Amsterdam.
PL	Physics Letters.
PM	Philosophical Magazine.
PNASI	Proceedings of the National Academy of Sciences, India.
PNASU	Proceedings of the National Academy of Sciences of the United States of America (Washington).
PNISI	Proceedings of the National Institute of Sciences of India.
PP	Photochemistry and Photobiology.
PPMSJ	Proceedings of the Physico-Mathematical Society of Japan.
PPS	Proceedings of the Physical Society, London.
PR	Physical Review.
Pramāṇa	Pramāṇa (India).
PRIA	Proceedings of the Royal Irish Academy.
PRL	Physical Review Letters.
PRR(Suppl.)	Philips Research Reports, Supplements.
PRS	Proceedings of the Royal Society of London.
PS	Physica Scripta.
PSS	Planetary and Space Science.
PTRSL	Philosophical Transactions of the Royal Society of London.
PZ	Physikalische Zeitschrift.
PZS	Physikalische Zeitschrift der Sowjetunion.
QR	Quarterly Reviews, Chemical Society.
RIHTR	Revue Internationale des Hautes Températures et des Réfractaires. Paris.
RiSc	La Ricerca Scientifica.
RJIC	Russian Journal of Inorganic Chemistry. - English translation of ZNK.
RJPC	Russian Journal of Physical Chemistry. - English translation of ZFK.
RMP	Reviews of Modern Physics.
RO	Revue d'Optique, Théorique et Instrumentale.

RPA	Revue de Physique Appliquée.
RR	Radiation Research.
RRP	Revue Roumaine de Physique.
RS	Ricerche Spettroscopiche, Laboratorio Astrofisico della Specola Vaticana.
SA	Spectrochimica Acta.
SA(Suppl.)	Spectrochimica Acta (Vol. <u>11</u>), Supplement (1957). Proceedings of the 6th Colloquium Spectroscopicum Internationale, Amsterdam, May 14-19, 1956.
SAAJ	Soviet Astronomy - AJ. - English translation of AZ.
SAJS	South African Journal of Science.
Science	Science.
Sci. Pap. IPCR (Tokyo)	Scientific Papers of the Institute of Physical and Chemical Research, Tokyo.
SCJ	Siberian Chemistry Journal. - English translation of ISOANK.
SJQE	Soviet Journal of Quantum Electronics. - English translation of KEM.
SL	Science of Light (Tokyo).
SPJ	Soviet Physics Journal. - English translation of IVUZF.
SpL	Spectroscopy Letters.
SPU	Soviet Physics - Uspekhi. - English translation of UFN.
TA	Thermochimica Acta.
TFS	Transactions of the Faraday Society.
TVT	Teplofizika Vysokikh Temperatur. - For English translation see HT(USSR).
UFN	Uspekhi Fizicheskikh Nauk. - For English translation see SPU.
USIP	University of Stockholm, Institute of Physics. Reports.
VMUK	Vestnik Moskovskogo Universiteta (Seriya II), Khimiya. - For English translation see MUCB.
ZA	Zeitschrift für Astrophysik.
ZAMP	Zeitschrift für Angewandte Mathematik und Physik. [Journal for Applied Mathematics and Physics (ZAMP)].
ZE	Zeitschrift für Elektrochemie. Berichte der Bunsengesellschaft für Physikalische Chemie.
ZFK	Zhurnal Fizicheskoi Khimii. - For English translation see RJPC.
ZN	Zeitschrift für Naturforschung.
ZNK	Zhurnal Neorganicheskoi Khimii. - For English translation see JIC(USSR) [1956-1958] and RJIC [1959+].
ZP	Zeitschrift für Physik.
ZPC	Zeitschrift für Physikalische Chemie.
ZPS	Zhurnal Prikladnoi Spektroskopii. - For English translation see JAS.
ZWP	Zeitschrift für wissenschaftliche Photographie, Photophysik und Photochemie.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
($107, 109$)Ag₂		$(\mu = 53.947829_3) \quad D_0^0 = 1.66 \text{ eV}^a$								OCT 1974 A
E	40159.1	146.0 ₈	H	1.54				E \leftarrow X, R	40135.7 H	(5)(7)(8)
D	$1_{\Pi_u}(1_u)$ 39023.7	166.7	H ^R	1.13 ₄				D \leftarrow X, R	39010.7 ^b H ^R	(5)(8)
C	$1_{\Pi_u}(1_u)$ 37626.9	172.9	H ^Q	1.0 ₇				C \leftarrow X, R	37617.0 ^c H ^Q	(5)(7)(8)
B	35827.3	151.3	H	0.70				B \leftrightarrow X, R	35806.7 H	(5)(8)
A	22996.4	154.6	H	0.587 ^d				A \leftrightarrow X, R	22977.5 ₀ H	(1)(2)* (5)
X	$1_{\Sigma_g^+}$ 0	192.4	H	0.643 ^d						
$^{107}\text{Ag}^{27}\text{Al}$		$\mu = 21.5440781 \quad D_0^0 = 1.9_5 \text{ eV}^a$								OCT 1974
C	1_{Π} 31744.8	[221.06] ^b		[0.1225] ^c		[1.6]	[2.525]	C \leftarrow X, R	31727.33 ^c Z	(2)
B	1_{Σ^+} 27459.1 ₇	[199.85]	Z (1.6 ₆)	0.11706 ^d	0.00112	1.6	2.5854	B \leftarrow X, R	27432.32 Z	(2)
X	1_{Σ^+} 0	[254.34]	Z (1.1 ₃)	0.12796	0.00076	1.27	2.4728			
(107)Ag^{197}Au		$(\mu = 69.294807_5) \quad D_0^0 = 2.0_6 \text{ eV}^a$ Four bands in thermal emission, possibly forming a progression with $\omega \approx 200 \text{ cm}^{-1}$. No wavelengths given.								OCT 1974 (1)
$^{109}\text{Ag}^{209}\text{Bi}$		$\mu = 71.594910_6$								FEB 1975 A
B (0^+)	20753.0	145.29	H	0.335 ^a				B \leftrightarrow X, R	20749.6 H	(1)(2)(3)*
A (0^+)	16364	144.0		0.53	(0.0200) ^b	(0.0000551)	(0.0153)	A \rightarrow X, R	16360 ^c	(2)(3)*
X' (1)	4185	148.5		0.50	(0.0199) ^b	(0.0000483)	(0.0143)	A \rightarrow X', R _V	12176.8 H ^Q	(3)*
X (0^+)	0	152.14	H	0.405 ^d	(0.0198) ^b	(0.0000435)	(0.0135)			

Ag₂:
^aThermochemical value (mass-spectrom.)(3)(4)(6),
 recalculated (9).
^bQ head at 38995.6 cm⁻¹.
^cR head at 37628.2 cm⁻¹.
^dConstants for ¹⁰⁷Ag/¹⁰⁹Ag; $w_e y_e(A) = +0.0023$, $w_e y_e(X) = +0.0003$.
 (1) Ruamps, CR 238, 1489 (1954).
 (2) Kleman, Lindkvist, AF 2, 385 (1955).
 (3) Drowart, Honig, JCP 25, 581 (1956); JPC 61, 980 (1957).
 (4) Schissel, JCP 26, 1276 (1957).
 (5) Ruamps, AP(Paris) 4, 1111 (1959).
 (6) Ackerman, Stafford, Drowart, JCP 33, 1784 (1960).
 (7) Maheshwari, IJP 37, 368 (1963).
 (8) Choong, Wang, Lim. Nature 209, 1300 (1966).
 (9) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

AgAl:
^aThermochemical value (mass-spectrom.)(1).
^bFrom (2), no details.
^cConstants refer to the normal ¹⁰⁷Ag/¹⁰⁹Ag isotopic mixture.
^dPerturbations in v=0 and 1.
 (1) Blue, Gingerich, 16th Annual Conference on Mass Spectrometry and Allied Topics, Pittsburgh (May 1968); paper 129.
 (2) Clements, Barrow, TFS 64, 2893 (1968).

AgAu: ^aThermochemical value (mass-spectrom.)(2).
 (1) Ruamps, SA(Suppl.) 11, 329 (1957).
 (2) Ackerman, Stafford, Drowart, JCP 33, 1784 (1960).
 AgBi: ^a $w_e y_e = +0.00007$.
^bRotational structure not resolved. The rotational constants have been estimated (3) from the appearance of extra heads in the red and infrared systems. They appear doubtful considering the unexpectedly large values of r_e resulting from them.
^cHead of the 0-0 band at 16394.5 cm⁻¹.
^d $w_e y_e = +0.00044$.
 (1) Houdart, Lochet, CR B 271, 38 (1970).
 (2) Lochet, CR B 272, 44, 797 (1971); 274, 174 (1972).
 (3) Lochet, JP B 7, 505, L543 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{109}\text{Ag}^{81}\text{Br}$										
		$\mu = 46.423560_9$ $D_0^0 = 3.1 \text{ eV}^a$ Fragments of a band system at 24000 cm^{-1} , in absorption.								OCT 1974
C	43537.4	205.0	H 0.74					C \leftarrow X, R	43516.0 H	(3) (4)
B (0^+)	31280.4 ₃	180.8	H 4.45 ^b					B \leftrightarrow X, R	31246.0 ₂ H	(1)(8) (1)* (2)
X $1\Sigma^+$	0	247.7 ₂	H 0.679 ₅	0.063407 ₃	0.0002282 ₂ ^c	1.7	2.39309	Microwave sp. ^d		(7)(9)
$^{107}\text{Ag}^{35}\text{Cl}$										
		$\mu = 26.3497888$ $D_0^0 = 3.22 \text{ eV}^a$ (290) Fragments of two progressions. Continuous absorption above 47500 cm^{-1} .								OCT 1974
D	(48800)	294.1	H 1.70					D \leftarrow X, R		(4) (4)
C	43525.7	278.36	Z 4.047 ^c	0.11912 ₇	0.001492 ^d	9.40 ^e	2.3174 ₂	C \leftarrow X, R	43500.9 ^b H	(4)
B 0^+	31602.65	343.49	Z 1.17	0.12298388	0.00059540 ₅ ^f	6.305 ₄ ^g	2.280792	B \leftrightarrow X, R	31569.32 Z	(1)* (2)(3) (5)(8) (9)
X $1\Sigma^+$	0							Microwave sp. ^h		(6)(7)(11)
$^{(107)}\text{Ag}^{(63)}\text{Cu}$										
		$(\mu = 39.612012_7)$ $D_0^0 = 1.7_6 \text{ eV}^a$								OCT 1974
B	25851.6	178.5	H 0.50					B \rightarrow X, R	25825.0 H	(3)
A	20836	171.5	H <0.5					A \rightarrow X, R	20806 H	(1)
X	0	231.8	H 0.80							
$^{107}\text{Ag}^{19}\text{F}$										
		$\mu = 16.1316107$ $D_0^0 = 3.6_4 \text{ eV}^a$ Unclassified bands, $\nu \geq 38400 \text{ cm}^{-1}$. Continuous absorption at 33000 cm^{-1} .								OCT 1974
C								C \leftarrow X, R		(3)(5) (3)(5)
B 0^+	(31663)	[373.6]	H ^b	[0.25548 ₆]	^c	[47.2]	[2.0224 ₄]	B \leftarrow X, R	31594.13 Z	(1)(3)(5)*
A 0^+	(29220)	[455.39]	Z ^d	[0.27268]	0.00593 ^d	[37.1] ^e	[1.9576]	A \leftarrow X, V	29250.87 Z	(3)(5)*
X $1\Sigma^+$	0	513.447	Z 2.593	0.2657020	0.0019206 ^f	28.4 ^f	1.983179	Microwave sp. ^g		(4)

AgBr: ^aThermochemical value (5)(6).

^b $\omega_{ey_e} = -0.060$.

^c $\gamma_e = +1.6_0 \times 10^{-7}$. (9) give constants for $^{107}\text{Ag}^{79}\text{Br}$.

^dFor values of $\text{eqQ}(^{79}\text{Br}, ^{81}\text{Br})$ see (7)(9).

- (1) Brice, PR 38, 658 (1931).
- (2) Mulliken, PR 51, 310 (1937).
- (3) Metropolis, Beutler, PR 55, 1113 (1939).
- (4) Barrow, Mulcahy, Nature 162, 336 (1948).
- (5) Brewer, Lofgren, JACS 72, 3038 (1950).
- (6) Barrow, JCP 22, 573 (1954).
- (7) Krisher, Norris, JCP 44, 974 (1966).
- (8) Davidovits, Bellisio, JCP 50, 3560 (1969).
- (9) Hoeft, Lovas, Tiemann, Törring, ZN 26 a, 240 (1971).

AgCl: ^aThermochemical value (10).

^b0-0 band not observed.

^c $\omega_{ey_e} = -0.38_6$. The vibrational levels converge rapidly above $v=4$.

^d $+ [6.2(v+\frac{1}{2})^2 - 2.9(v+\frac{1}{2})^3] \times 10^{-5}$ (for $v \leq 4$).

^e $- [0.0257(v+\frac{1}{2}) - 0.467(v+\frac{1}{2})^2] \times 10^{-8}$ (for $v \leq 4$).

^f $\gamma_e = +6.28_1 \times 10^{-7}$.

^g $\beta_e = -0.0018 \times 10^{-8}$; $H_e = -0.9_7 \times 10^{-14}$.

^h $\mu_{el} = 5.7_0$ D [(6), criticised by (11) for neglect of quadrupole hfs]. For value of $\text{eqQ}(^{35}\text{Cl})$ see (11).

- (1) Brice, PR 35, 960 (1930).
- (2) See ref. (1) of AgBr.
- (3) See ref. (2) of AgBr.
- (4) Jenkins, Rochester, PR 52, 1141 (1937).
- (5) Barrow, Morgan, Wright, PCS (1959), p. 303.
- (6) Krisher, Norris, JCP 44, 391 (1966).
- (7) Pearson, Gordy, PR 152, 42 (1966).

AgCl (continued):

(8) Clements, Barrow, TFS 63, 2876 (1967).

(9) Davidovits, Bellisio, JCP 50, 2787 (1969).

(10) Hildenbrand, JCP 52, 5751 (1970).

(11) Hoeft, Lovas, Tiemann, Törring, ZN 26 a, 240 (1971).

AgCu: ^aThermochemical value (mass-spectrom.)(2).

(1) Ruamps, SA(Suppl.) 11, 329 (1957).

(2) Ackerman, Stafford, Drowart, JCP 33, 1784 (1960).

(3) Joshi, Majumdar, PPS 78, 197 (1961).

AgF: ^aThermochemical value (2). In agreement with an upper limit ($D_0^0 < 3.70$ eV) from predissociation in $A\ 0^+$ (3)(5).

^bFrom band heads: $\Delta G(3/2, 5/2, 7/2) = 380.3, 373.2, 356.9$.

^cLevels with $v \geq 1$ are predissociated.

^dPredissociation in $v=0$ for $J > 85$ and in $v=1$ for $J > 40$.

Levels with $v > 1$ are not observed.

^e $D_1 = 67.3 \times 10^{-8}$; $H_0 = -3.2 \times 10^{-12}$.

^f $\gamma_e = +3.8_0 \times 10^{-6}$; $\beta_e = +0.1 \times 10^{-8}$.

^g $\mu_{el}(v=0) = 6.2_2$ D.

- (1) Joshi, Sharma, IJPAP 1, 86 (1963).
- (2) Zmbov, Margrave, JPC 71, 446 (1967).
- (3) Clements, Barrow, CC (1968), p. 27.
- (4) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 35 (1970).
- (5) Barrow, Clements, PRS A 322, 243 (1971).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
($^{107}\text{Ag}^{(69)}\text{Ga}$)										
A	33061.1	$(\mu = 41.906769_3)$ 153.2	H	$D_0^0 = 1.8_7 \text{ eV}^a$ 0.8 ₂				A \leftarrow X,	R 33045.3	H (1)* OCT 1974
X ($^1\Sigma$)	0	184.7	H	0.6 ₅						
($^{107}\text{Ag}^1\text{H}$)										
c_0 ($^3\Pi_0$)		$(\mu = 0.99841289)$ [5.10] ^b		$D_0^0 = 2.28 \text{ eV}^a$ [6.0]				$c_0\leftarrow$ X,	R 46981.1	Z (10)* OCT 1974
d $^3\Sigma^+$				[(3.83)] ^c				(46875) ^d		(10)*
c_1 $^3\Pi_1$				[(4.95)] ^e				$c_1\leftarrow$ X,	R (46600) ^e	(10)*
D $^1\Pi$ (46720)		[844.7]	Z (120)	5.23 ^f	0.58			D \leftarrow X,	R 46360.9	Z (10)*
b ($^3\Delta_1$) 1				[4.805] ^g				b \leftarrow X, ^h	R 44529.2	Z (10)*
B $^1\Sigma^+$ (44512)		[(1089)] ⁱ	(65)	(4.87) ⁱ	(0.31)			B \leftarrow X,	R (44234) ⁱ	(10)
a $^3\Pi_r$ (41700) ^j		(1450)	(50)	(>6.3) ^j						(10)
C $^1\Pi$ (41261)		(1589) ^k	(42) ^k	[6.54]	(0.31) ^k			C \leftarrow X,	41173.6	Z (10)*
A $^1\Sigma^+$ 29959		[1489.6]	Z 87.0 ^l	[6.090 ₅]	0.348 ₅ ^l			A \leftrightarrow X,	R 29897.9 ₄	Z (2)(3)* (5) (6)(8)
X $^1\Sigma^+$ 0		1759.9	Z 34.06 ^m	6.449 ^o	0.201 ^m					
($^{107}\text{Ag}^2\text{H}$)										
d $^3\Sigma^+$		$(\mu = 1.97685802)$ [(2.09)] ^c		$D_0^0 = 2.31 \text{ eV}^p$ [(2.02)]				(47019) ^d		(10) OCT 1974
c_2 ($^3\Pi_2$) (47025)		[644.7]	Z (29)	2.36 ^q	0.12			$c_2\leftarrow$ X, ^r	R 46748.1	Z (10)*
c_1 ($^3\Pi_1$) (46939)		[(716.0)] ^s	(32)	(2.58) ^s	(0.13)			$c_1\leftarrow$ X,	R (46700) ^s	(10)*
D $^1\Pi$		Constants for $v=1$:		2.35 ^f				D \leftarrow X,	R 47160.3	Z (10)
b ($^3\Delta_1$) 1				[2.468] ^g				b \leftarrow X, ^h	R 44600.5	Z (10)
B $^1\Sigma^+$ (44476)		[(811)] ⁱ	(36)	(2.52) ⁱ	(0.12)			B \leftarrow X,	R (44287.0) ⁱ	(10)*
a $^3\Pi_r$ (41700) ^j		(1040)	(25)	(>3.2) ^j						(10)
C $^1\Pi$ (41269)		(1108) ^k	(25)	[3.335]	(0.118) ^k			C \leftarrow X,	V_R 41195.5	Z (10)*
A $^1\Sigma^+$ 29960.0 ₄		1160.82	31.73 ^l	3.154	0.100 ^l			A \rightarrow X,	R 29911.22	Z (4)(6)(7)*
X $^1\Sigma^+$ 0		1250.70	Z 17.17	3.2572	0.0722					

AgGa: ^aThermochemical value (mass-spectrom.)(2).

(1) Biron, CR B 264, 1097 (1967).

(2) Gingerich, Blue, 18th Annual Conference on Mass Spectrometry and Allied Topics, San Francisco (June 1970); paper F2.

Ag¹H, Ag²H:

^aGraphical Birge-Sponer extrapolation of X ¹Σ⁺. Thermochemical value 2.4₉ eV (1).

^bStrong perturbations. Constants valid near J=0 only.

^cFrom perturbations in c₁(v=0).

^dEstimated energy of v'=0, N'=0 relative to X ¹Σ(v=0, N=0).

^eThe only observed level is strongly perturbed by more than one state. Constants refer to unperturbed region around J=19. Origin of 0-0 band (not observed) at 46692 cm⁻¹.

^fPerturbations in v=0, 1; bands going to v'=0 of Ag²H have not been analyzed. Constants refer to unperturbed regions near J=0. Large Λ-type doubling;

Ag¹H: Δv_{ef}(v=0) = +0.244 J(J+1) - ...

Ag²H: Δv_{ef}(v=1) = +0.077₂ J(J+1).

^gConstants refer to unperturbed region near J=0. Large Ω-type doubling;

Ag¹H: Δv_{ef} = +0.156 J(J+1) - ...

Ag²H: Δv_{ef} = +0.033₇ J(J+1) + ...

^hP branch very weak or absent.

ⁱApproximate constants for the deperturbed state. Origins of the 0-0 bands at 44225.0 cm⁻¹ (Ag¹H) and 44277.4 cm⁻¹ (Ag²H). v=1 is free of perturbations;

Ag¹H: B₁ = 4.412, D₁ = 3.5 × 10⁻⁴, v₀(1-0) = 45322.8 cm⁻¹;

Ag²H: B₁ = 2.343, D₁ = 0.95 × 10⁻⁴, v₀(1-0) = 45097.8 cm⁻¹.

^jConstants estimated from perturbations in C ¹Π, B ¹Σ⁺,

Ag¹H, Ag²H (continued):

D ¹Π of Ag¹H, and b 1 of Ag²H; vibrational numbering uncertain. +150 ≤ A ≤ +200.

^kApproximate constants for the deperturbed state. Perturbations in v=0, 1, 2 are caused by a ³Π. ΔG(1/2, 3/2) = 1519, 1453 (Ag¹H); 1056, 987 (Ag²H).

^lAnomalous potential curve; see (6). Constants for higher vibrational levels of Ag¹H in (2)(3). The constants for Ag²H (w_ey_e = -1.94₂, γ_e = -0.009) are valid for v ≤ 4.

^mHigher order terms are needed to represent levels with v ≥ 4; see (2)(3)(5).

n_{H0} = +88 × 10⁻¹⁰ (Ag¹H); +6 × 10⁻¹⁰ (Ag²H).

^oRKR potential curve (9).

^pFrom the value for Ag¹H.

^qConstants refer to unperturbed regions near J=0. Small Λ-type doubling.

^rR, P much weaker than Q branches.

^sApproximate constants for the deperturbed state. v=0 strongly perturbed by more than one state. Origin of 0-0 band (not observed) at 46794 cm⁻¹.

(1) Farkas, ZPC B 5, 467 (1929).

(2) Bengtsson-Knave, Olsson, ZP 72, 163 (1931).

(3) Bengtsson-Knave, NARSSU (IV) 8(4) (1932).

(4) Koontz, PR 48, 138 (1935).

(5) Gerö, Schmid, ZP 121, 459 (1943).

(6) Learner, PRS A 269, 327 (1962).

(7) Ringström, AF 21, 145 (1962).

(8) Loginov, OS(Engl. Transl.) 16, 220 (1964).

(9) Singh, Rai, CJP 43, 1685 (1965).

(10) Ringström, Åslund, AF 32, 19 (1966).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$(^{107})\text{Ag}^{165}\text{Ho}$		$(\mu = 64.862383) \quad D_0^0 = 1.2_6 \text{ eV}^a$								NOV 1974
$^{107}\text{Ag}^{127}\text{I}$		$\mu = 58.024719_5 \quad D_0^0 = 2.6 \text{ eV}^a$								NOV 1974
D	(45487)	(176) ^b	H (2.5)					D \leftarrow X, R		(3)(6)
C	44721	155.5 ^c	H 1.7					C \leftarrow X, R 44695	H	(3)(6)
		Continuous absorption above 42400 cm^{-1} .								(3)
		Continuous absorption $29800 - 33300 \text{ cm}^{-1}$, maximum at 31500 cm^{-1} .								(1)(2)(12)
B	0^+ 31194.06	127.14	Z 4.255 ^d	0.040716	0.000572 ^d	[2.19] ^e	2.6712	B \leftrightarrow X, R 31153.42	Z	(1)* (2)(5) (7)(10)(11)
		Continuous absorption above 24000 cm^{-1} .								(4)
A	23906	151.2	H					A \leftarrow X, R 23879	H	(4)
X	$1\Sigma^+$ 0	206.52	Z 0.445	0.04486806	0.0001413 ₉ ^f	0.847 ^g	2.544621	Microwave sp. ^h		(13)
$(^{107})\text{Ag}^{115}\text{In}$		$(\mu = 55.380129_3) \quad D_0^0 = 1.6_9 \text{ eV}^a$								NOV 1974
B	33535.52	140.66 ^b	H 0.462					B \leftarrow X, R 33527.91 ^b	H	(2)
A	32471.41	133.20 ^c	H 0.377					A \leftarrow X, R 32460.41 ^c	H	(1)
X	(1Σ) 0	155.54 ^d	H 0.423							
$(^{107})\text{Ag}^{(7)}\text{Li}$		$(\mu = 6.5839134) \quad D_0^0 = 1.81 \text{ eV}^a$								APR 1975
$(^{107})\text{Ag}^{23}\text{Na}$		$(\mu = 18.920867_7) \quad D_0^0 = 1.40 \text{ eV}^a$								NOV 1974
$^{107}\text{Ag}^{16}\text{O}$		$\mu = 13.9132446_1 \quad D_0^0 = 2.2_9 \text{ eV}^a$								NOV 1974 A
		Unclassified band system in the red; no details.								(1)
B	$2_{II} \begin{cases} 3/2 & x_2+28113.8 \\ 1/2 & x_1+28072.3 \end{cases}$	539.1 ^b	H 6.1 ₅	[0.3195]		[50]	[1.947 ₄]	B \rightarrow X, V	28137.3 ^b H	(2)*
		535.7 ^b	H 6.3 ₄	[0.3178] ^{bc}		[51] ^b	[1.952 ₆]		28094.2 ^b H	
		[241.1] ^b	H d	[0.2816] ^d		[171]	[2.074]		24416.0 ^b H	
A	$2_{II} \begin{cases} 3/2 & x_2+24540 \\ 1/2 & x_1+24370 \end{cases}$	[237.3] ^b	H d	[0.2812] ^{cd}		[168]	[2.076]	A \rightarrow X, R	24244.5 ^b H	(2)*

AgHo: ^aThermochemical value (mass-spectrom.)(1).
(1) Cocke, Gingerich, JPC 75, 3264 (1971).

AgI: ^aThermochemical value (8)(9).
^bAnalysis (3) uncertain. (6) estimate $v_e \approx 46000$,
 $\omega_e \approx 165$.

^cAverage of (3) and (6).

^dFrom $v=0,1,2$ only; $\gamma_e = -0.000031$. The vibrational levels converge rapidly to a maximum in the potential curve at $\sim 510 \text{ cm}^{-1}$ above $v=0$; see (7).

^e $D_1 = 2.53 \times 10^{-8}$, $D_2 = 3.38 \times 10^{-8}$.

^f $\gamma_e = +5.7 \times 10^{-8}$.

^gCalculated from $4B_e^3/\omega_e^2$. From the rotational analysis of B-X bands $D_0 \dots D_2 = 0.96, 0.90, 0.85, 0.84_0 \times 10^{-8}$.

^hFor value of eqQ(127I) see (13).

- (1) Brice, PR 38, 658 (1931).
- (2) Mulliken, PR 51, 310 (1937).
- (3) Metropolis, PR 55, 636 (1939).
- (4) Metropolis, Beutler, PR 55, 1113 (1939).
- (5) Sastry, Rao, IJP 19, 136 (1945).
- (6) Barrow, Mulcahy, Nature 162, 336 (1948).
- (7) Barrow, Mulcahy, PPS 61, 99 (1948).
- (8) Brewer, Lofgren, JACS 72, 3038 (1950).
- (9) Barrow, JCP 22, 573 (1954).
- (10) Barrow, Morgan, Wright, PCS (1959), p. 303.
- (11) Barrow, Clements, Wright, TFS 63, 2874 (1967).
- (12) Davidovits, Bellisio, JCP 50, 3560 (1969).
- (13) Hoeft, Lovas, Tiemann, Törring, ZN 26 a, 240 (1971).

AgIn: ^aThermochemical value (mass-spectrom.)(3).

^bFor $^{107}\text{AgIn}$.

^cFor $^{109}\text{AgIn}$.

^dAverage for $^{109}\text{AgIn}$ (from $A \leftarrow X$) and $^{107}\text{AgIn}$ (from $B \leftarrow X$).

(1) Biron, CR B 265, 1026 (1967).

(2) Biron, CR B 265, 1427 (1967).

(3) Gingerich, Blue, 18th Annual Conference on Mass Spectrometry and Allied Topics, San Francisco (June 1970); paper F2.

AgLi: ^aThermochemical value (mass-spectrom.)(1).

(1) Neubert, Zmbov, JCS FT I 70, 2219 (1974).

AgNa: ^aThermochemical value (mass-spectrom.)(1).

(1) Piacente, Gingerich, HTS 4, 312 (1972).

AgO: ^aThermochemical value (mass-spectrom.)(4).

^bFor the natural isotopic mixture $^{107}\text{Ag}/^{109}\text{Ag}$.

^cThe Ω -type doubling observed in the $\frac{1}{2} \rightarrow \frac{1}{2}$ transitions of $A \rightarrow X$ and $B \rightarrow X$ is approximately given by $0.029(J+\frac{1}{2}) - \dots$ and $0.022(J+\frac{1}{2}) - \dots$, respectively.

^dPredissociation above $v=0$, $J=66\frac{1}{2}$ in $A \ ^2\Pi_{1/2}$ and above $v=0$, $J=73\frac{1}{2}$ in $A \ ^2\Pi_{3/2}$. No bands involving $v'=2$ have been observed.

(continued p. 17)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{107}\text{Ag}^{160}$ (continued)										
X	$2_{II}\begin{cases} 3/2 \\ 1/2 \end{cases}$	x_2^e x_1^e	490.5^b H 490.2^b H	2.8_6 3.0_6	0.3036 0.3020^c	0.0026 0.0025	50 45	1.997_7 2.003_0		
$(^{107}\text{Ag}^{(32)}\text{S})$		$(\mu = 24.6115147) \quad D_0^0 = 2.2_1 \text{ eV}^a$								NOV 1974
$(^{107}\text{Ag}^{(121)}\text{Sb})$		$(\mu = 56.737174_8)$								NOV 1974
System A:		{ Strong 0-0 sequence of R shaded bands in thermal emission; $w_e' - w_e'' = -13.1 \text{ cm}^{-1}$. Vibr. numbering of 0-1 and 0-2 sequences uncertain. ^a						16330.1	H	(1)
System B:		{ Strong 0-0 sequence of V_R shaded bands in thermal emission; $w_e' - w_e'' = -9.5 \text{ cm}^{-1}$, $w_e' x_e' - w_e'' x_e'' = +0.107 \text{ cm}^{-1}$. ^a						15654.2	H ^Q	(1)
$(^{107}\text{Ag}^{(80)}\text{Se})$		$(\mu = 45.730700_7) \quad D_0^0 = 2.0_6 \text{ eV}^a$								NOV 1974
B	(41491)	$([183])^b$	H					B \leftarrow X,	R (41465) ^b	H (1)
A	(29436)	$([127])^b$	H					A \leftarrow X,	R (29382) ^b	H (1)
(X)	0	$(234)^b$	H							
$(^{107}\text{Ag}^{(120)}\text{Sn})$		$(\mu = 56.515625_7) \quad D_0^0 = 1.3_8 \text{ eV}^a$								NOV 1974
$(^{107}\text{Ag}^{(130)}\text{Te})$		$(\mu = 58.644313_8) \quad D_0^0 = 1.9_9 \text{ eV}^a$								NOV 1974
C	41079	138.0	H	2.50				C \leftarrow X,	R 41050	H (1)
B	38765	146.2	H	0.20				B \leftarrow X,	R 38740	H (1)
A	29168	124.0	H	0.01				A \leftarrow X,	R 29132	H (1)
X	0	195.3	H	0.30						

AgO (continued):

^eNot quite certain that this is the ground state. It appears to be regular with $A \approx +135 \text{ cm}^{-1}$, contrary to expectations; see (3).

- (1) Loomis, Watson, PR 48, 280 (1935).
- (2) Uhler, AF 7, 125 (1954).
- (3) Cheetham, Barrow, AdHTC 1, 7 (1967).
- (4) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

AgS, AgSe, AgTe:

^aThermochemical value (mass-spectrom.)(2).

^bAnalysis uncertain.

- (1) Maheshwari, PPS 81, 514 (1963).
- (2) See ref. (4) of AgO.

AgSb: ^aAccording to (1) the bandhead measurements refer to $^{109}\text{Ag}^{121}\text{Sb}$.

- (1) Lefebvre, Lochet, CR B 275, 85 (1972).

AgSn: ^aThermochemical value (mass-spectrom.)(1).

- (1) Ackerman, Drowart, Stafford, Verhaegen, JCP 36, 1557 (1962).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{27}\text{Al}_2$										
		$\mu = 13.4907703$ $D_0^0 = 1.5_5 \text{ eV}^a$								NOV 1975
A $^3\Sigma_u^-$	17269.3 ₆	278.80 ^b	H 0.831 ^c	0.1907	0.0013	3.9	2.560	A \rightarrow X, R	17234.0 ₅ H	(1)* (2)*
X $^3\Sigma_g^-$	0	350.01 ^b	H 2.022 ^d	0.2054	0.0012	3.0 ₇	2.466			
$^{27}\text{Al}^{79}\text{Br}$										
		$\mu = 20.1070892$ $D_0^0 = 4.4_3 \text{ eV}^a$								NOV 1975 A
A $^1\Pi$	35879.5	297.2	H ^Q 6.40 ^b	0.1555 ^c	0.00216 ^d	1.8 ^e	2.322	A \leftrightarrow X, R	35837.8 H ^Q	(1)(2)* (3) (4)* (5)
a $^3\Pi_1$	23779.3	410.32	H ^Q 1.75	0.164 ^f	0.001		2.26	a \rightarrow X, V	23795.3 H ^Q	(4)(6)*
$^3\Pi_0$	23647	411.2	(Z) 1.75						23663 ^g (Z)	
X $^1\Sigma^+$	0	378.0	H ^Q 1.28	0.15919713	0.00086044 ₉ ^h	1.1285 ⁱ	2.294807 ^j	Microwave sp. ^k		(9)
AlC										
The spectrum originally attributed to AlC (1) was later shown (2) to be due to Al ₂ .										NOV 1975
$^{27}\text{Al}^{35}\text{Cl}$										
		$\mu = 15.2301459$ $D_0^0 = 5.12 \text{ eV}^a$								NOV 1975 A
Fragments of additional systems in the region 48200 - 54900 cm^{-1} .										
b ($^3\Sigma$)	(43591)	(350) ^b		[0.226] ^c			[2.21]	b \rightarrow a, R	18847.40 H ^Q 18911 (Z) 18975.00 H ^Q	(7) (5)*
A $^1\Pi$	38254.0	449.96	H ^Q 4.37 ^d	0.259 ^e	0.006		2.06 ₇	A \leftrightarrow X, R _V	38237.7 H ^Q	(1)* (2)(3) (4)
a $^3\Pi_r$	$\begin{cases} 24658 \\ 24593.84 \\ 24528 \end{cases}$	524.35	H ^Q 2.175	0.250 ^f	0.002		2.10	a \rightarrow X, V	24680 (Z) 24615.31 H ^Q 24541.65 H ^P	(5)*
X $^1\Sigma^+$	0	481.30	H ^Q 1.95	0.24393012	0.00161113 ^g	2.502 ₇ ^h	2.130113 ⁱ	Microwave sp. ^j		(9)(11)

Al_2 : ^aThermochemical value (mass-spectrom.)(5). Values in (3)(4) are somewhat higher.
^bFrom (1) who wrongly attributed the spectrum to AlC .
^c $w_e y_e = -0.0104$.
^d $w_e y_e = -0.0105$.
(1) Zeeman, CJP 32, 9 (1954).
(2) Ginter, Ginter, Innes, ApJ 139, 365 (1964).
(3) Blue, Gingerich, 16th Annual Conference on Mass-Spectrometry and Allied Topics, Pittsburgh (1968);
(4) Uy, Drowart, TFS 67, 1293 (1971). | paper 129.
(5) Stearns, Kohl, HTS 5, 113 (1973).

$AlBr$: ^aThermochemical value (8); 4.58 eV from prediss. in $A^1\Pi$.
^b $w_e y_e = -0.527$. This state may have a potential hump of ~ 0.20 eV (7)(8).
^cPredissociation for $v > 3$. According to (11) emission
^d $r_e = -0.000175$. | from $v=2, 3$ breaks off at $J=93, 67$, resp..
^eRapidly increasing with v .
^fEstimated from P and Q head separations.
 ϵ_P head at 23657.9 cm^{-1} .
 $h r_e = +2.030 \times 10^{-6}$.
ⁱ $\beta_e = -0.00207 \times 10^{-7}$; $H_e = -1.119 \times 10^{-14}$.
^jFrom the corrected $B_e = 0.15920431$.
^kFor values of eqQ see (10).
(1) Crawford, Ffolliott, PR 44, 953 (1933).
(2) Howell, PRS A 148, 696 (1935).
(3) Mahanti, IJP 2, 369 (1935).
(4) Miescher, HPA 8, 279 (1935); 9, 693 (1936).
(5) Jennergren, Nature 161, 315 (1948); AMAF A 35,
(6) Sharma, ApJ 113, 219 (1951). | No. 22 (1948).
(7) Barrow, TFS 56, 952 (1960).
(8) Barrow, Nature 189, 480 (1961).

$AlBr$ (continued):

- (9) Wyse, Gordy, JCP 56, 2130 (1972).
(10) Hoeft, Törring, Tiemann, ZN 28 a, 1066 (1973).
(11) Ram, Upadhyaya, Rai, Singh, OPA 6, 38 (1973).

AlC : (1)(2) See ref. (1)(2), respectively, of Al_2 .

$AlCl$: ^aThermochemical value [see Appendix of ref.(10)]. See also
^bEstimated from observed isotope shifts. | (8).
^c $v > 0$ probably predissociated.
^d $w_e y_e = -0.216$. This state may have a potential hump of
^ePredissociation in $v=10$ (3). | ~ 0.26 eV (6)(8).
^fEstimated from P and Q head separations.
 $\epsilon + 4.697 \times 10^{-6}(v+\frac{1}{2})^2 - 5.7 \times 10^{-9}(v+\frac{1}{2})^3$.
 $h \beta_e = -0.0053 \times 10^{-7}$; $H_e = -4.456 \times 10^{-14}$.
ⁱFrom the corrected $B_e = 0.24394229$.
^j $\mu_{el} = 1$ to 2 D (9). Values of eqQ in (9)(12).
(1) Bhaduri, Fowler, PRS A 145, 321 (1934).
(2) Mahanti, ZP 88, 550 (1934).
(3) Holst, ZP 93, 55 (1934); Dissertation (Stockholm,
(4) See ref. (4) of $AlBr$. | 1935).
(5) Sharma, ApJ 113, 210 (1951).
(6) Barrow, JCP 22, 573 (1954).
(7) Reddy, Rao, CJP 35, 912 (1957).
(8) See ref. (7) of $AlBr$.
(9) Lide, JCP 42, 1013 (1965); 46, 1224 (1967) (erratum).
(10) Hildenbrand, Theard, JCP 50, 5350 (1969).
(11) See ref. (9) of $AlBr$.
(12) See ref. (10) of $AlBr$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{27}\text{Al}^{19}\text{F}$		$\mu = 11.1484740$ $D_0^0 = 6.8_9 \text{ eV}^a$ I.P. = 9.8 eV^b								MAR 1976 A	
Unclassified V shaded bands in the region $70900 - 74600 \text{ cm}^{-1}$, in absorption.											(6)*
H $1\Sigma^+$	67320	958	H 7.0	[0.59214]		[8.3]	[1.5980]	H→B, V 13114.57 Z		(17)(26)	
								H→A, V 23447.32 ^c Z		(17)(26)	
g $3\Sigma^+$	(66910)			[0.59544]		[9.51]	[1.5936]	H←X, V 67397.03 Z		(5)(6)*	
G $1\Sigma^+$	66334.0	[931.46]	Z 8.0 H	0.60490	0.00767 ^d	[10.26]	1.5811	g→b, V 22177.12 Z		(23)(26)	
								G→B, V 12123.34 Z		(26)	
								G→A, V 22456.09 ^c Z		(9)* (26)	
								G←X, V 66405.81 Z		(5)(6)*	
f 3Π	65803	[938.90]	Z (5.9)	0.59355 ^{ef}	0.00480	[9.29]	1.5961	f→c, V 10853.84 ^c Z		(26)	
								f→b, V 21072.71 ^c Z		(17)(23)(26)	
								f→a, V 38576.1			
								38623.6		(7)(10)	
								38670.9			
F 1Π	65795.6	955.33	Z 5.38	0.59281 ^{gf}	0.00459	[8.78]	1.5971	F→B, V 11589.46 ^c Z		(9)* (26)	
								F→A, V 21922.22 ^c Z		(9)* (26)	
								F←X, V 65871.95 ^c Z		(5)(6)*	
e $3\Sigma^+$	(65010)			[0.59464]		[8.4]	[1.5946]	e→c, V 10064.76 Z		(23)(26)*	
								e→b, V 20283.63 Z		(17)(23)(26)	
E 1Π	63689.4	923.02	Z 5.28	0.58709 ^h	0.00464	[9.46]	1.6049	E→A, V 19799.95 ^c Z		(17)(26)	
								E←X, V 63749.68 ^c Z		(5)(6)	
d (3Δ) ⁱ	(63203)	[930.2]	(Z)					d→a, V 36017.6 (Z)		(7)(10)	
D 1Δ ⁱ	61229.5	901.05	Z 6.11	0.58297	0.00502	[9.87]	1.6105	D→A, V 17328.85 ^c Z		(4)(9)* (26)	

A&F: ^aThermochemical value, see Appendix of ref. (20), also (21).

^bInterpretation of Rydberg states (26). Electron impact appearance potentials vary from 9.5 to 10.1 eV (16)(19)(21).

^cBand origins as defined in (26); add $B''\Lambda''^2 - B'\Lambda'^2$ to obtain zero lines.

^dConstants from (26). Small discrepancy with the B_1 value in the same paper.

^e Λ -type doubling $\Delta v_{fe} = + 0.00338 \times N(N+1)$.

^fInteractions between levels of $F^1\Pi$ and $f^3\Pi$.

^g Λ -type doubling $\Delta v_{fe}(v=0) = + 0.00559 \times J(J+1) - \dots$, decreasing with increasing v .

^h Λ -type doubling $\Delta v_{fe} = + 0.00025 \times J(J+1)$.

ⁱCompare with ab initio calculations by (28).

(continued p. 22)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{27}\text{Al}^{19}\text{F}$ (continued)										
C $1\Sigma^+$	57688.0	938.22	Z 5.09 ^j	0.58992	0.00458 ^k	9.23 ^l	1.6010	C→A, V	13806.16 ^c Z	(2)(3)* (4) (26)
c $3\Sigma^+$	54957.7	933.66	Z 4.81	0.58861 ^m	0.00457	9.8	1.6028	C↔X, V	57755.89 Z	(5)(6)(11) (13)
								c→b, V	10218.89 Z	(23)(26)
								c→a, V	27722.2 27769.8 27817.1	(4)* (10) (26)
B $1\Sigma^+$	54251.0	866.6 ₀	Z 7.4 ₅ ⁿ	0.57968	0.00560	[10.49]	1.6151	B↔X, V	54282.46 Z	(5)(6)* (11) (13)(26)
b $3\Sigma^+ i$	44813.2 ^o	786.37	Z 7.64 ^p	0.56280 ^{mq}	0.00651 ^r	11.5	1.6391	b→a, ν_R	17503.4 17550.9 17598.2	(4)(23)(26)
A $1\Pi i$	43949.2	803.9 ₄	Z 5.99 ^s	0.55640 ^{tq}	0.00534 ^u	10.56 ^v	1.6485	A↔X, ν_R	43949.73 ^c Z	(1)* (2)(3) (4)* (5) (12)(25)
a $3\Pi_r i$	27241 ^w	827.8	Z 3.9	0.5570 ₃	0.00453	[9.82]	1.6476	a→X,	27254	(29)
X $1\Sigma^+ i$	0	802.2 ₆	Z 4.77	0.5524798	0.0049841 ^x	10.464 ^y	1.654369	Microwave sp. ^z		(18)(22)(24)

A&F (continued):

$$^j \omega_e y_e = -0.017.$$

$$^k y_e = -0.000011.$$

$$^l H_e \approx -1.1 \times 10^{-12}.$$

^mMagnetic hyperfine structure; very small spin splitting.

$$^n \omega_e y_e = -0.04_5.$$

^oRelative energies of singlet and triplet states derived from the analysis of spin-forbidden perturbations, see ^q.

$$^p \omega_e y_e = -0.009.$$

^qInteractions between levels of A 1Π and b $3\Sigma^+$ (26).

$$^r y_e = -0.00002.$$

^s $\omega_e y_e = -0.050$. This state may have a potential maximum of ~ 0.35 eV; see e.g. (15).

^t Λ -type doubling $\Delta \nu_{fe} = +0.00010 \text{ J}(J+1)$.

$$^u y_e = -0.000043.$$

A1F (continued);

$$v_{He} \approx -2.0 \times 10^{-12}.$$

$$w_A = +47 \text{ cm}^{-1}.$$

$$x + 1.718 \times 10^{-5} (v + \frac{1}{2})^2 + 4.7 \times 10^{-8} (v + \frac{1}{2})^3. \text{ From (24);}$$

slightly different constants in (22).

$$y \beta_e = -0.015 \times 10^{-7}.$$

$$z \mu_{el} = 1.53 \text{ D (18). For eqQ(A1) see (22)(24)(27).}$$

Additional constants derived from Zeeman effect measurements (g_J , mol. quadrupole moment, etc.) in (27).

- (1) Rochester, PR 56, 305 (1939).
- (2) Naudé, Hugo, PR 90, 318 (1953).
- (3) Naudé, Hugo, CJP 31, 1106 (1953).
- (4) Rowlinson, Barrow, PPS A 66, 437 (1953).
- (5) Rowlinson, Barrow, PPS A 66, 771 (1953).
- (6) Barrow, Rowlinson, PRS A 224, 134 (1954).
- (7) Dodsworth, Barrow, PPS A 67, 94 (1954).
- (8) Gross, Hayman, Levi, TFS 50, 477 (1954).
- (9) Naudé, Hugo, CJP 32, 246 (1954).
- (10) Dodsworth, Barrow, PPS A 68, 824 (1955).
- (11) Naudé, Hugo, CJP 33, 573 (1955).
- (12) Barrow, Johns, Smith, TFS 52, 913 (1956).

- (13) Naudé, Hugo, CJP 35, 64 (1957).
- (14) Witt, Barrow, TFS 55, 730 (1959).
- (15) Barrow, TFS 56, 952 (1960).
- (16) Porter, JCP 33, 951 (1960).
- (17) Barrow, Kopp, Scullman, PPS 82, 635 (1963).
- (18) Lide, JCP 38, 2027 (1963); 42, 1013 (1965).
- (19) Ehlert, Blue, Green, Margrave, JCP 41, 2250 (1964).
- (20) Hildenbrand, Murad, JCP 44, 1524 (1966).
- (21) Murad, Hildenbrand, Main, JCP 45, 263 (1966).
- (22) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 1029 (1970).
- (23) Kopp, Barrow, JP B 3, L118 (1970).
- (24) Wyse, Gordy, Pearson, JCP 52, 3887 (1970).
- (25) Liszt, Smith, JQSRT 12, 947 (1972).
- (26) Barrow, Kopp, Malmberg, PS 10, 86 (1974); USIP Report 74-15 (March 1974).
- (27) Honerjäger, Tischer, ZN 29 a, 342 (1974).
- (28) So, Richards, JP B 7, 1973 (1974).
- (29) Rosenwaks, Steele, Broida, CPL 38, 121 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{27}\text{Al}^1\text{H}$										
c $3\Pi_r$ b 3Σ a $3\Pi_r$ E 1Π D $1\Sigma^+$ C $1\Sigma^+$ A 1Π X $1\Sigma^+ n$	a^d	$\mu = 0.97153602$		$D_0^0 < 3.06 \text{ eV}^a$ b [6.759] ^c [6.704] [5.620] ^e [6.56] ^f 6.664 ^h 6.3869 ^{ijkl} 6.3907						NOV 1975 A (15)* (5)(9) (7)(26) (13)(26)* (3)(11)(13) (17)* (1)(13)* (11)(13) (17)* (2)(4)(6)* (8)(10)(13)* (14)(16)* (20)(25)

Al^1H , Al^2H :

- ^aFrom the predissociation in $A^1\Pi$ (10)(12). The most recent theoretical calculations for Al^1H (28) recommend 3.05 eV.
- ^b $v=0$ perturbed.
- ^cPerturbation at $N=19$, predissociation at $N>25$.
- ^d(22) estimate $a \approx 12000 \text{ cm}^{-1}$. $A = +40.2$.
- ^eConstants for the f component. Large Λ -type doubling, Δv_{fe} positive; J.W.C. Johns [see (26)] reports a new $^1\Sigma^+$ state just above $E^1\Pi$. Predissociation for $J>12$ (?) (26).
- ^fPerturbed at $J=5$, predissociated for $J>10$.
- ^gFrom $\Delta G(\frac{1}{2})$ of the hydride and deuteride.
- ^hPerturbations.
- ⁱ $D_1 = 10 \times 10^{-4}$.
- ^j Λ -type doubling, $\Delta v_{ef}(v=0) = +0.0097 J(J+1) - \dots$.
- ^kPredissociation by rotation in $v=0,1$ (Al^1H) and $v=0,1,2$ (Al^2H); this state has a potential maximum (12) of $\sim 0.15 \text{ eV}$ (18).
- ^lZeeman effect (21).
- ^m $D_1 = 11.20 \times 10^{-4}$; also higher order constants (16).
- ⁿFor theoretical calculations concerning the ground state of AlH see (23)(24)(27)(28).
- ^o $w_e y_e = +0.239$.
- ^p $y_e = +0.00161$.
- ^q $\beta_e = -0.047 \times 10^{-4}$.
- ^r $0 < A < 12$.
- ^s $v=0$ perturbed. $v=1$ ($B_1 = 2.938$, $D_1 = 3 \times 10^{-5}$) predissociated at $N \approx 16$ and perturbed in $^3\Pi_0$.
- ^tConstants for the f component. The e component interacts with $G^1\Sigma^+$.
- ^uApproximate deperturbed value; interaction with the e component of $E^1\Pi$.

^v Λ -type doubling, $\Delta v_{ef} = +0.0020 J(J+1)$.

^w $y_e = -0.052$.

^x $D_1 = 2.21 \times 10^{-4}$, $D_2 = 6.96 \times 10^{-4}$.

^y $w_e y_e = +0.098$.

^z $y_e = +0.00055$.

- (1) Bengtsson, Hulthén, ZP 52, 275 (1929).
- (2) Farkas, ZP 70, 733 (1931).
- (3) Bengtsson-Knave, NARSSU 8, No. 4 (1932).
- (4) Farkas, Levy, ZP 84, 195 (1933).
- (5) Holst, ZP 86, 338 (1933).
- (6) Holst, Hulthén, ZP 90, 712 (1934).
- (7) Holst, ZP 90, 728 (1934).
- (8) Holst, ZP 90, 735 (1934).
- (9) Challacombe, Almy, PR 51, 930 (1937).
- (10) Olsson, Dissertation (Stockholm, 1938).
- (11) Grabe, Hulthén, ZP 114, 470 (1939).
- (12) Herzberg, Mundie, JCP 8, 263 (1940).
- (13) Nilsson, Dissertation (Stockholm, 1948); AMAF A 35, No. 19 (1948).
- (14) Kleman, Lagercrantz, Uhler, AF 2, 359 (1950).
- (15) Kleman, AF 6, 407 (1953); Dissertation (Stockholm, 1953).
- (16) Zeeman, Ritter, CJP 32, 555 (1954).
- (17) Khan, PPS 71, 65 (1958).
- (18) Hurley, PRS A 261, 237 (1961).
- (19) Khan, PPS 79, 745 (1962).
- (20) Loginov, OS(Engl. Transl.) 16, 220 (1964).
- (21) Klynning, Neuhaus, AF 28, 249 (1965).
- (22) Grimaldi, Lecourt, Lefebvre-Brion, Moser, JMS 20, 341 (1966).
- (23) Cade, Huo, JCP 47, 649 (1967).

(continued p. 27)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{27}\text{Al}^1\text{H}^+$										
A $2\Pi_r$	(27686) ^a (27593)	(1770)		6.851 ^b	0.248	41	1.591 ₄	A \rightarrow X, V	27760.2 Z 27667.8 Z	DEC 1975 (1)* (2)
X $2\Sigma^+$	0	(1620)		6.763 ^c	0.398	47	1.601 ₈			
$^{27}\text{Al}^{127}\text{I}$										
A 1Π		$\mu = 22.2507434$ $D_0^0 = 3.77 \text{ eV}^a$						A \leftarrow X, 31487 ^b	DEC 1975 A (1)*	
a $\begin{cases} 3\Pi_1 \\ 3\Pi_0 \end{cases}$	22089.5 21889.3	333.4 H 2.0 337.2 H 2.0						a \leftrightarrow X, V V _R 21899.6 H	(1)*	
X $1\Sigma^+$	0	316.1 H 1.0		0.11769985	0.000558586 ^c	d	2.53710 ₂	Microwave sp. ^e		(3)
$^{27}\text{Al}^{14}\text{N}$										
A $3\Pi_i$	a	$\mu = 9.21869147$						A \rightarrow X, V	19727.37 Z	DEC 1975 (1)*
(X) $3\Pi_i$ ^d	e	[746.93] Z		[0.5811] ^{bc} 0.5730 ^b	0.0056		[0.139] [1.7739] [0.136] 1.7864			

Al^1H , Al^2H (continued):

- (24) Cade, Bader, Henneker, Keaveny, JCP 50, 5313 (1969).
- (25) Huron, Physica 41, 58 (1969).
- (26) Lagerqvist, Lundh, Neuhaus, PS 1, 261 (1970).
- (27) Laws, Stevens, Lipscomb, JCP 54, 4269 (1971).
- (28) Meyer, Rosmus, JCP 63, 2356 (1975).

Al^1H^+ : $a_A = +108$.

^b(2) finds breaking-off in P and R at $N=28$ ($v=0$).

^cSpin splitting constant $f \approx +0.06$.

- (1) Almy, Watson, PR 45, 871 (1934).
- (2) Holst, ZP 89, 40 (1934).

AlI : ^aFrom the analysis of fluctuation bands (2).

^bVertical transition from $v''=0$.

$$c + 1.0477 \times 10^{-6} (v + \frac{1}{2})^2 - 2.46 \times 10^{-9} (v + \frac{1}{2})^3.$$

$$d_{D_v} = [6.5212 - 0.00957 (v + \frac{1}{2})] \times 10^{-8}; H_e = -4.590 \times 10^{-15}.$$

^eValues of eqQ_v ($v=0...3$) in (4).

- (1) Miescher, HPA 8, 279 (1935); 9, 693 (1936).
- (2) Barrow, TFS 56, 952 (1960).
- (3) Wyse, Gordy, JCP 56, 2130 (1972).
- (4) Törring, Tiemann, Hoeft, ZN 28 a, 1062 (1973).

AlN : ^a $A_0 = -23.0$.

^bAll lines in the $^3\Pi_2 - ^3\Pi_2$ and high J lines in the $^3\Pi_0 - ^3\Pi_0$ subbands are broad ($\sim 0.15 \text{ cm}^{-1}$), probably on account of unresolved nuclear hyperfine structure.

^cPredissociation near $J=48$.

^dNot certain that this is the ground state.

$$e A_0 = -33.0, A_1 = -34.5.$$

- (1) Simmons, McDonald, JMS 41, 584 (1972).

State	T _e	w _e		w _e x _e	B _e	α _e	D _e (10 ⁻⁶ cm ⁻¹)	r _e (Å)	Observed Transitions		References
									Design.	ν ₀₀	
²⁷Al¹⁶O											
μ = 10.0419507 ₁ D ₀ ⁰ = 5.27 ± 0.04 eV ^a I.P. = 9.5 ₃ eV ^b											
Additional states and transitions predicted by (43).											
F 2Σ ⁺	[47677.3]			[0.5088]		[2.15]	[1.816 ₄]	F→A, R	41843.52 Z 41972.36 Z	(44)*	
E 2Δ _i c	45562 ^d 45431	(503)		[0.4951] [0.4919]		[1.9]	[1.844 ₄]	E↔A, R	39979.81 Z 39977.17 Z	(4)(25)(28)* (31)*	
D 2Σ ⁺ c	40266.7	819.6	Z 5.8	0.5652 ^e	0.0046 ^f	1.10	1.723 ₄	(D→B), ^g R	(19552)	(30)	
								D↔A, V	34841.23 Z 34970.09 Z	(4)(25)(28)* (23)* (25) (31)(32)* (39)(40)(45)	
								D↔X, R	40187.2 Z	(10)(18)* (4)(10)* (12)(25) (26)* (29)	
C 2Π _r c	33153 33079	856	H 6	h				(C→B), ⁱ R _V	(12457) (12383)	(1)(2)* (3)* (6)* (7)* (9) (11)(14)(15) (16)(17)* (21)* (24) (25)(30)(31)* (33)(36)(37)	
								C↔X, R	33092 33018	(33)(51)	
B 2Σ ⁺ j	20688.95	870.05	Z 3.52	0.6040 ₈ ^k	0.0044 ₇	1.16	1.6670	B ^l ↔X, R	20635.22 Z		
A 2Π _i j	5470.6 ^m 5341.7	728.5	H 4.15	[0.5374] ^{no} [0.5333] ^o		[1.1]	[1.7708]	A↔X, ^p R	5346 5217		
X 2Σ ⁺ j	0	979.23	Z 6.97	0.6413 ₆ ^{qr}	0.0058 ₀	1.08 ^s	1.6179	IR ^t and ESR ^u sp.			

A10: ^aLower limit from the laser fluorescence study of A10 formed in the reaction $\text{Al} + \text{O}_2$ (49), upper limit from the re-interpretation (28)(41) of the long-wavelength limit of an absorption continuum (25). Good agreement with the most recent mass-spectrometric results (34)(42); slightly lower value by flame photometry (48). Further references

reviewed in (49).

^bElectron impact appearance potential (13)(22)(42).

^cTheoretical calculations concerning these states in (43).

^d $A_0 = -64.8$.

^eSpin splitting constant $\gamma = +0.0060$ (50).

^f $\gamma_e = -0.00005$.

A40 (continued):

- ^gUncertain observation. See also (43).
- ^hRotational constants in (10) are unreliable; see (29).
Perturbations.
- ⁱUncertain identification (18). See also (43).
- ^jTheoretical calculations concerning these states (46)(47).
- ^kSpin splitting constant $\gamma = -0.0074$ (50), disagreeing with +0.020 in (6)(10).
- ^lRadiative lifetime $\tau = 102$ ns (49), 127 ns (35). The corresponding B-X oscillator strengths, $f_{00} = 0.027$ and 0.021, resp., are compared in (49) with additional experimental and theoretical (38)(46) results. Relative b. strengths (27).
- ^m $A_0 = -127.8$.
- ⁿ Λ -type doubling $\Delta v_{fe} = -0.0128(J+\frac{1}{2})$.
- ^oSlightly different constants in (44).
- ^pTheoretical oscillator strengths in (46).
- ^qSpin splitting constant $\gamma_0 = +0.0050$ (50), smaller than earlier values (6)(10) and in better agreement with ESR (33) and theoretical (50) results.
- ^rPerturbations (5)(9) by $A^2\Pi_1$ (28).
- ^s $\beta_e = +0.02 \times 10^{-6}$.
- ^tAbsorption f-number for the IR fundamental band 0.000033 (52). Theoretical values in (46)(47)(52).
- ^uIn rare gas matrices at 4 K (33).
- (1) Pomeroy, PR 29, 59 (1927).
- (2) Sen, IJP 11, 251 (1937).
- (3) Roy, IJP 13, 231 (1939).
- (4) Coheur, Rosen, BSRSL 10, 405 (1941).
- (5) Rosen, PR 68, 124 (1945).
- (6) Lagerqvist, Nilsson, Barrow, PPS A 62, 356 (1956);
AF 12, 543 (1957).
- (7) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

- (8) Gurvich, Veits, IANSF 22, 673 (1958). For engl. transl. see BASPS 22, 670 (1958).
- (9) Shimauchi, SL 7, 101 (1958).
- (10) Goodlett, Innes, Nature 183, 243 (1959).
- (11) Loginov, OS(Engl. Transl.) 6, 67 (1959); 16, 220 (1964).
- (12) Bécart, Declerck, CR 251, 2153 (1960).
- (13) Drowart, De Maria, Burns, Inghram, JCP 32, 1366 (1960).
- (14) Nicholls, JRNBS A 66, 227 (1962).
- (15) Tawde, Korwar, PPS 80, 794 (1962).
- (16) Bécart, Mahieu, CR 256, 5533 (1963); JP(Paris) 25, 873 (1964).
- (17) Edse, Rao, Strauss, Mickelson, JOSA 53, 436 (1963).
- (18) Tyte, Nature 202, 383 (1964).
- (19) Hébert, Tyte, PPS 83, 629 (1964).
- (20) Tyte, Hébert, PPS 84, 830 (1964).
- (21) Tyte, Nicholls, IAMS 1 (1964).
- (22) Burns, JCP 44, 3307 (1966).
- (23) Krishnamachari, Narasimham, Singh, CJP 44, 2513 (1966).
- (24) Sharma, JQSRT 7, 283, 289 (1967).
- (25) Tyte, PPS 92, 1134 (1967).
- (26) Mahieu, Bécart, CSp 13, 95 (1968).
- (27) Linton, Nicholls, JQSRT 9, 1 (1969).
- (28) McDonald, Innes, JMS 32, 501 (1969).
- (29) McDonald, Innes, Goodlett, Tolbert, JMS 32, 511 (1969).
- (30) Prasad, Narayan, IJPAP 7, 413 (1969).
- (31) Singh, Narasimham, JP B 2, 119 (1969).
- (32) Singh, PIAS A 71, 82 (1970).
- (33) Knight, Weltner, JCP 55, 5066 (1971).
- (34) Farber, Srivastava, Uy, JCS FT I 68, 249 (1972).
- (35) Johnson, Capelle, Broida, JCP 56, 663 (1972).

(continued p. 31)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{27}\text{Al}^{31}\text{P}$		$\mu = 14.4200754$ $D_0^0 = 2.2_0 \text{ eV}^a$							DEC 1975	
$^{27}\text{Al}^{(32)}\text{S}$		$(\mu = 14.6327889)$ $D_0^0 = 3.84 \text{ eV}^a$							DEC 1975	
C $^2\Sigma^+$	(35797)	[430.0]	H (14)	0.2402 ^b	0.0036	3.1	2.190	C \leftarrow X, R 35714.9	(2)	
B ($^2\Pi$)	(30104) (29986)	[530]	Strong perturbations.					B \leftarrow X, R 30061 29943	H H (2)(4)	
A $^2\Sigma^+$	23433.80	510.9 ₁	Z 1.45	0.2461 ^{cd}	0.0012	2.1	2.164	A \leftrightarrow X, R 23381.16	Z (1)* (2)(4)	
X $^2\Sigma^+$	0	617.1 ₂	Z 3.33	0.2799 ^e	0.0018	2.2	2.029		(6)*	
$^{27}\text{Al}^{(80)}\text{Se}$		$(\mu = 20.1712814)$ $D_0^0 = 3.4_6 \text{ eV}^a$							DEC 1975	
A ($^2\Sigma$)	23183.5	389.8	H 1.23					A \leftrightarrow X, R 23144.8	H (2)	
X ($^2\Sigma$)	0	467.6	H 2.08							
$^{27}\text{Al}^{(28)}\text{Si}$		$(\mu = 13.7351103)$ $D_0^0 = 2.3_4 \text{ eV}^a$							DEC 1975	
$^{27}\text{Al}^{(130)}\text{Te}$		$(\mu = 22.3412584)$ $D_0^0 = 2.7_3 \text{ eV}^a$							DEC 1975	

AlO (continued):

- (36) Gole, Zare, JCP 57, 5331 (1972).
- (37) Liszt, Smith, JQSRT 12, 947 (1972).
- (38) Michels, JCP 56, 665 (1972).
- (39) Singh, JQSRT 12, 1343 (1972).
- (40) Tawde, Tulasigeri, JP B 5, 1681 (1972).
- (41) Drowart, private communication (1973).
- (42) Hildenbrand, CPL 20, 127 (1973).
- (43) Schamps, CP 2, 352 (1973).
- (44) Singh, JP B 6, 521 (1973).
- (45) Singh, Saksena, PIAS A 77, 139 (1973).
- (46) Yoshimine, McLean, Liu, JCP 58, 4412 (1973).
- (47) Das, Janis, Wahl, JCP 61, 1274 (1974).
- (48) Frank, Krauss, ZN 29 a, 742 (1974).
- (49) Dagdigian, Cruse, Zare, JCP 62, 1824 (1975).
- (50) Mahieu, Jacquinet, Schamps, Hall, JP B 8, 308 (1975).
- (51) Rosenwaks, Steele, Broida, JCP 63, 1963 (1975).
- (52) Sulzmann, JQSRT 15, 313 (1975).

AlP: ^aThermochemical value (mass-spectrom.)(1).

- (1) De Maria, Gingerich, Malaspina, Piacente, JCP 44, 2531 (1966).

AlS: ^aThermochemical value (mass-spectrom.)(3)(5).

^bPredissociation for $v \geq 2$.

^cSpin splitting constant $\gamma_0 \approx -0.0055$ (6).

AlS (continued):

^dSmall perturbations (4)(6).

^eSpin splitting constant $\gamma_0 \approx +0.0045$ (6).

- (1) McKinney, Innes, JMS 3, 235 (1959).
- (2) Mal'tsev, Shevelkov, Krupnikov, OS(Engl. Transl.) Suppl. No. 2, 4 (1966).
- (3) Ficalora, Hastie, Margrave, JPC 72, 1660 (1968).
- (4) Kronekvist, Lagerqvist, AF 32, 133 (1969).
- (5) Uy, Drowart, TFS 67, 1293 (1971).
- (6) Lavendy, Mahieu, Bécart, CJS 18, 13 (1973); Lavendy, Jacquinet, CJS 20, 141 (1975).

AlSe: ^aThermochemical value (mass-spectrom.)(1)(3).

- (1) See ref. (3) of AlS.
- (2) Singh, Tewari, Mohan, JP B 2, 627 (1969); IJPAP 10, 386 (1972).
- (3) See ref. (5) of AlS.

AlSi: ^aThermochemical value (mass-spectrom.)(1).

- (1) Stearns, Kohl, HTS 5, 113 (1973).

AlTe: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1) See ref. (3) of AlS.
- (2) See ref. (5) of AlS.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{40}\text{Ar}_2$		$\mu = 19.9811921$ $D_0^0 = 0.01051 \text{ eV}^a$ Unclassified, mostly diffuse absorption bands in the regions 88100 - 90100, 106600 - 108200, 113000 - 113900, 114900 - 127200 cm^{-1} . Fragments of a system of very diffuse absorption bands.								DEC 1975 A	
H		[128.4] ^{bc}	H	Long upper state progressions.				H \leftarrow X, V	(117666) ^b 112033.9 ^{bc}	(13)	
G		[170.5] ^{bc}	H					G \leftarrow X, V	110930.9 ^{bc}	(13)*	
F	(0_u^+)	[134.2] ^b	H					F \leftarrow X, V	108492.2 ^b	(13)	
E		[170] ^b	H	All bands appear diffuse.				E \leftarrow X, V	107330 ^b	(13)	
D		[183.2] ^b	H	All bands appear diffuse.				D \leftarrow X, V	106029.5 ^b	(13)	
C	(0_u^+) 95033.0	67.0	H	4.03 ^d				C \leftarrow X, V	95050.7	(13)*	
B	($1_{\Sigma_u^+}$) 0_u^+	[136.49] ^e	Z		[0.1057] ^e	[7] ^e	[2.82 ₅] ^e	B \leftarrow X, V	93241.26 ^e	(13)* (24)	
A	($3_{\Sigma_u^+}$) 1_u	[133.7] ^b	H	f				A \leftrightarrow X, V	92393.3 ^b	(13)*	
		Emission continuum longward of 1067 \AA (93750 cm^{-1}); maxima near 93000 and 79000 cm^{-1} , the former exhibiting oscillatory structure (2)(10)(23) extending to 67000 cm^{-1} (21). The emission originates from the lowest excited states [see (12)] and at 79000 cm^{-1} is characterized by radiative lifetimes of 3.2 μs (1_u ?) and 4.2 ns (0_u^+ ?) (20); see also (22). Additional continua at 65000, 53000, 47000 cm^{-1} (1)(4)(7)(9), and diffuse emission bands in the region 87000 - 89000 cm^{-1} (1)(2).						A, B \rightarrow X		(1)* (3)* (5)(6)	
X	$1_{\Sigma_g^+}$	0	[25.74]	Z	ξ	0.05975	0.00375 ^h	[11.3] ⁱ	3.758	j	(18)(24)
$^{40}\text{Ar}_2^+$		$\mu = 19.9810550$ $D_0^0 \geq 1.049 \text{ eV}^a$ Theoretical calculations, applied to scattering data (4)(4b)(4c)(5).								DEC 1975 A	
X	$2_{\Sigma_u^+}$	0						2.43 (theor.)			

Ar₂: ^aCalculated by (24) from spectroscopic data for the five lowest vibrational levels in X ¹Σ_g⁺ and using information from long-range forces and from the second virial coefficient. D_e = 99.55 cm⁻¹; compare with earlier results by (11)(14)(15)(16)(17)(19).

^bLowest observed level and interval; vibrational numbering unknown.

^cThe vibrational levels assigned to G and H may belong to a single state with ω_e ≥ 176, ω_ex_e ≈ 2.85.

^dThis state correlates with 4s[¹/₂]₁ + ¹S.

^eConstants for the lowest of four rotationally analyzed levels (24); vibrational numbering unknown, (21) estimate v=22. This state correlates with 4s[³/₂]₁ + ¹S and may have a potential hump of ~70 cm⁻¹ (13).

^fRapid convergence to the limit 4s[³/₂]₂ + ¹S.

^gΔG(³/₂, ..., ²/₂) = 20.41, 15.60, 10.91, 6.78. G(0) = 14.80.

^hγ_e = - 0.000313.

ⁱD₁, ..., D₅(10⁻⁷cm⁻¹) = 16.6, 20, 33, 52, 200.

^jRaman spectrum (15a)(21a)(22a).

- (1) Tanaka, JOSA 45, 710 (1955).
- (2) Tanaka, Jursa, LeBlanc, JOSA 48, 304 (1958).
- (3) Tanaka, Huffman, Larrabee, JQSRT 2, 451 (1962).
- (4) Strickler, Arakawa, JCP 41, 1783 (1964).
- (5) Huffman, Larrabee, Tanaka, AO 4, 1581 (1965).
- (6) Wilkinson, CJP 45, 1715 (1967).
- (7) Verkhovtseva, Fogel, Osyka, OS(Engl. Transl.) 25, 238 (1968).
- (8) Wilkinson, CJP 46, 315 (1968).
- (9) Hurst, Bortner, Strickler, PR 178, 4 (1969).
- (10) Michaelson, Smith, CPL 6, 1 (1970).
- (11) Cavallini, Gallinaro, Meneghetti, Scoles, Valbusa, CPL 7, 303 (1970).
- (12) Mulliken, JCP 52, 5170 (1970).

Ar₂ (continued):

- (13) Tanaka, Yoshino, JCP 53, 2012 (1970).
- (14) Barker, Fisher, Watts, MP 21, 657 (1971).
- (15) Maitland, Smith, MP 22, 861 (1971).
- (15a)Morgan, Frommhold, PRL 29, 1053 (1972).
- (16) Parson, Siska, Lee, JCP 56, 1511 (1972).
- (17) Le Roy, JCP 57, 573 (1972).
- (18) Docken, Schafer, JMS 46, 454 (1973).
- (19) Present, JCP 58, 2659 (1973).
- (20) Keto, Gleason, Walters, PRL 33, 1365 (1974).
- (21) Michaelson, Smith, JCP 61, 2566 (1974).
- (21a)Frommhold, JCP 61, 2996 (1974); 63, 1687 (1975).
- (22) Oka, Rao, Redpath, Firestone, JCP 61, 4740 (1974).
- (22a)Frommhold, Bain, JCP 63, 1700 (1975).
- (23) Verkhovtseva, Yaremenko, Fogel, Ovechkin, Katrunova, OS(Engl. Transl.) 38, 98 (1975).
- (24) Colbourn, Douglas, JCP 65, 1741 (1976).

Ar₂⁺: ^aDifference between the ionization potential of Ar and the appearance potential of Ar₂⁺, the latter obtained as the longest-wavelength absorption line of Ar which produces photoionization (2). Similar results by electron impact; see ref. in (2)(3). Ar⁺-on-Ar scattering data indicate D_e = 1.30 eV (4a)(4b), consistent with theoretical (4) and semiempirical (3) calculations.

- (1) Aberth, Lorents, PR 144, 109 (1966).
- (2) Huffman, Katayama, JCP 45, 138 (1966).
- (3) See ref. (12) of Ar₂.
- (4) Gilbert, Wahl, JCP 55, 5247 (1971).
- (4a)Lorents, Olson, Conklin, CPL 20, 589 (1973).
- (4b)Mittmann, Weise, ZN 29 a, 400 (1974).
- (4c)Jones, Conklin, Lorents, Olson, PR A 10, 102 (1974).
- (5) Sidis, Barat, Dhuicq, JP B 8, 474 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{40}\text{Ar}(^{35})\text{Cl}$		$(\mu = 18.6496153_\mu)$ Continuous emission with strongest peak near 57250 cm^{-1} and additional maxima of decreasing intensity at higher energies; from chemiluminescent reactions (1)(2). Estimated constants for the strongly bound upper state: $T \approx 56800$, $w \approx 230 \text{ cm}^{-1}$, $D[\text{Ar}(^3\text{P}_2) - \text{Cl}] \approx 4.51 \text{ eV}$. Additional weaker emission at longer wavelengths (2).							JAN 1976 (2)	
$^{40}\text{Ar}^{19}\text{F}$		$\mu = 12.8767196$ Continuous emission with strongest peak near 52550 cm^{-1} and additional peaks of decreasing intensity at higher energies; from chemiluminescent reactions (2). Estimated constants for the strongly bound upper state: $T \approx 54300$, $w \approx 280 \text{ cm}^{-1}$, $D[\text{Ar}(^3\text{P}_2) - \text{F}] \approx 4.81 \text{ eV}$. Additional weaker emission in the region $35700 - 50000 \text{ cm}^{-1}$ (2).							JAN 1976 A (2)	
$^{40}\text{Ar}^{19}\text{F}^+$		$D_0^0 \geq 1.67 \text{ eV}^a$							JAN 1976	
$^{40}\text{Ar}^1\text{H}$ B 2_{Π} A $2_{\Sigma}(+)$	a	$\mu = 0.98303375$ <div style="display: flex; justify-content: space-around; align-items: center;"><div style="text-align: center;">$\begin{bmatrix} [10.129]^b \\ [10.200]^d \end{bmatrix}$</div><div style="text-align: center;">$\begin{bmatrix} [5.03] \\ [5.31] \end{bmatrix}$</div><div style="text-align: center;">$\begin{bmatrix} [1.3012] \\ [1.2966] \end{bmatrix}$</div></div> For a theoretical calculation of the ground state potential ($D_e = 0.0042 \text{ eV}$, $r_e = 3.57 \text{ \AA}$) and a comparison with experimental scattering data see (2).						B \rightarrow A, ^c R 13024.5 Z	(1)* JAN 1976 A	
$^{40}\text{Ar}^2\text{H}$ B 2_{Π} A $2_{\Sigma}(+)$	a	$\mu = 1.91746222$ <div style="display: flex; justify-content: space-around; align-items: center;"><div style="text-align: center;">$\begin{matrix} (1990) \\ (2057) \end{matrix}$</div><div style="text-align: center;">$\begin{matrix} 5.3262^b \\ 5.3402^{\text{gd}} \end{matrix}$</div><div style="text-align: center;">$\begin{matrix} 0.1310 \\ 0.1399 \end{matrix}$</div><div style="text-align: center;">$\begin{matrix} 1.500^e \\ [1.440]^h \end{matrix}$</div><div style="text-align: center;">$\begin{matrix} 1.2848 \\ 1.2831 \end{matrix}$</div></div> B \rightarrow A, ^f R _v 13040.38 Z						(1)* JAN 1976		

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{40}\text{Ar}^1\text{H}^+$ $x^1\Sigma^+ \quad 0$				$D_0^0 \geq 2.65 \text{ eV}^a$			1.28 ^b			JAN 1976

ArCl: (1) Golde, Thrush, CPL 29, 486 (1974).
(2) Golde, JMS 58, 261 (1975).

ArF, ArF^+ :

^aFrom the observed exothermicity of the reaction
 $\text{F}_2^+ + \text{Ar} = \text{ArF}^+ + \text{F}$ (1).
(1) Berkowitz, Chupka, CPL 7, 447 (1970).
(2) See ref. (2) of ArCl.

Ar^1H , Ar^2H :

^a $A_0 = (-)2.0$; see (1).
^b Λ -type doubling; see (1). Small perturbations are evident in the hydride spectrum.
^c0-0 band only; diffuse lines.
^d $v=0$ of Ar^1H , and $v>0$ of Ar^2H , are predissociated, probably by interaction with the unstable $x^2\Sigma^+$ ground state; see (1).
^eFrom Q branches; $H_e = +1.34 \times 10^{-9}$.
^f0-0 sequence only. Lines are sharp in the 0-0 band, but become more diffuse as v increases.
^gSpin splitting $\Delta v_{12} = (+)[0.0369(N+\frac{1}{2}) - \dots]$.
^h $D_1 = 1.426 \times 10^{-4}$; $H_0 = +0.96 \times 10^{-9}$.

Ar^1H , Ar^2H (continued):

(1) Johns, JMS 36, 488 (1970).
(2) Wagner, Das, Wahl, JCP 60, 1885 (1974).

Ar^1H^+ : ^aFrom the observed exothermicity of the reaction
 $\text{H}_2^+ + \text{Ar} = \text{ArH}^+ + \text{H}$ (1). A higher limit, $D_0^0 \geq 3.40 \text{ eV}$, is suggested by a tentative interpretation (1) of chemi-ionization processes. H^+ -on-Ar scattering data [(3)(5), and ref. therein] give $D_e = 4.17 \text{ eV}$, in reasonable agreement with theoretical calculations (2)(4).
^bFrom proton-argon scattering data [(3)(5), and ref. therein]. Slightly larger values from theoretical calculations (2)(4).

(1) Chupka, Russell, JCP 49, 5426 (1968).
(2) Roach, Kuntz, CC (1970), p. 1336.
(3) Klingbeil, JCP 57, 1066 (1972).
(4) Sidis, JP B 5, 1517 (1972).
(5) Weise, BBPC 77, 578 (1973).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{40}\text{Ar}(^{84})\text{Kr}$		$(\mu = 27.0703037)$	$D_0^0 \text{ a}$							JAN 1976 A
X $1\Sigma^+$ 0										(1)
										(1)
										(1)
										(2)
$^{40}\text{Ar}(^{84})\text{Kr}^+$										JAN 1976
										(1)
$^{40}\text{Ar}^{16}\text{O}$		$\mu = 11.4229054_7$								JAN 1976 A
										(2)
										(4)
$^{40}\text{Ar}(^{132})\text{Xe}$		$(\mu = 30.6703362)$								JAN 1976 A
X $1\Sigma^+$ 0										

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{75}\text{As}_2$		$\mu = 37.460800_2$ $D_0^0 = 3.96 \text{ eV}^a$								JAN 1976
N	(72137)	[319]						$N \leftarrow X,$	72082	(8)
M	(69607)	[365]						$M \leftarrow X,$	69575	(8)
J								$J \leftarrow X,$	66133 66015	(8)
I								$I \leftarrow X,$	65432 65308	(8)
H	(61726)	[364] H						$H \leftarrow X,$ ^b	R 61694 H	(8)
		Unclassified absorption bands in the region 47000 - 55000 cm^{-1} .								(9)
G	(54586)	[377] ^c H						$G \leftarrow X,$ ^d	R 54560 H	(8)(9)
F	(52221)	[386] H						$F \leftarrow X,$ ^e	R 52200 H	(8)(9)
		Fragments of other electronic states in the region 42400 - 44500 cm^{-1} .								(11)
b ($^3\Pi_u$)		Only $v=0$ observed.						$b \rightarrow X,$	R 42006	(2)(3)(4)
B $^1\Sigma_u^+$	(40925)	[243.6] ^f Z		[0.0712] ^f			[2.5]	$B \leftrightarrow X,$	R 40832.2 Z	(1)(2)(4)* (6)(7)(10)
A $^1\Sigma_u^+$	(40349)	[260.3] ^{gh} Z		[0.07202] ^{gh}			[2.50]	$A \leftrightarrow X,$	R 40265.0 Z	(1)(2)(4)* (6)(7)(9) (10)(11)(12)
d ($^3\Pi_g$) 1_g	30818.8	336.7 H 1.36		0.09222	0.00033		2.209 ₀	$d \rightarrow c,$ ⁱ	V 16185.6 H 16348.4 H	(4)* (5)* (6)
a ($^3\Sigma_u^-$) 0_u^+	24641.2	337.0 H 0.83		0.08664	0.00030		2.279 ₀	$d \rightarrow X,$	R 30772.4 H	(5)* (6)
e	19914.7	330.0 H 0.90						$(a \rightarrow c),$ ^j	V (10100)	(5)*
								$a \rightarrow X,$ ^k	R 24595.0 H	(4)* (6)
								$e \rightarrow X,$	R 19865.0 ^l H	(6)
c $^3\Sigma_u^+ \begin{cases} 0_u^- \\ 1_u \end{cases}$	$\begin{cases} 14644.4 \\ 14481.6 \end{cases}$	$\begin{cases} 314.3 \\ 314.3 \end{cases}$ H $\begin{cases} 1.17 \\ 1.17 \end{cases}$		$\begin{cases} 0.08491 \\ 0.08471^m \end{cases}$	$\begin{cases} 0.00035 \\ 0.00035 \end{cases}$		$\begin{cases} 2.302_1 \\ 2.303_6 \end{cases}$	$c(1_u) \rightarrow X,$	R 14424.0	(6)
X $^1\Sigma_g^+$	0	429.55 H 1.117 ⁿ		0.10179	0.000333 ^o		2.1026			

As₂:
^aFrom the predissociation limit in A ¹Σ_u⁺ assuming dissociation into ⁴S + ²D without kinetic energy (4). Extrapolation of the ground state vibrational levels (observed to v=70, i. e. 80% of D₀⁰) gives 3.93 eV (3)(4).
^bSystem G←X of (8).
^cBands with v' ≥ 3 are diffuse.
^dSystem E←X of (8).
^eSystem f←X of (8).
^fAdditional ΔG(v+½) and B_v values (v ≤ 7) in (10). Strong perturbations.
^gAdditional ΔG(v+½) and B_v values (v ≤ 17) in (10)(11)(12). Strong perturbations produced by interaction with the B and, possibly, other states.
^hIn emission no bands with v' ≥ 10 are observed except those with v' = 14 (2). In absorption bands with v' ≥ 10 are observed (9)(11) but the lines in them are broad except those with v' = 14 which are sharp. The line width varies greatly as a function of J in bands with v' ≥ 10. There is clearly a predissociation limit at 42700 ± 100 cm⁻¹.
ⁱOriginally (4) attributed to As₂⁺. Recognized as being due to neutral As₂ by (5). The lower states are the two case "c" components of c ³Σ_u⁺ (6).
^jStrong system in the infrared (5), not analysed in detail.
^kSystem D→X of (4).
^l19855 in (6) appears to be erroneous.
^mΩ-type doubling, Δv_{fe} = (-)0.00018 x J(J+1).
ⁿω_ey_e = + 0.000139, ω_ez_e = - 0.00001958.
^or_e = - 2.8 x 10⁻⁷.

- (1) Gibson, MacFarlane, PR 46, 1059 (1934).
- (2) Almy, Kinzer, PR 47, 721 (1935).
- (3) Almy, JPC 41, 47 (1937).
- (4) Kinzer, Almy, PR 52, 814 (1937).
- (5) Mrozowski, Santaram, JOSA 57, 522 (1967).
- (6) Perdigon, D'Incan, CJP 48, 1140 (1970).
- (7) Perdigon, Martin, D'Incan, JMS 36, 341 (1970).
- (8) Donovan, Strachan, TFS 67, 3407 (1971).
- (9) Topouzkhanian, Sibai, SA A 28, 2197 (1972).
- (10) Martin, Perdigon, D'Incan, JMS 50, 45 (1974).
- (11) Sibai, Perdigon, Topouzkhanian, ZN 29 a, 429 (1974).
- (12) Martin, Figuet, Perdigon, JMS 57, 319 (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{75}\text{As}_2^+ ?$										JAN 1976
<p>The spectrum tentatively assigned to As_2^+ in (1) has been shown to be due to the $d \rightarrow c$ transition of the neutral molecule; see ⁱ of As_2.</p> <p>The authors of (2) have described two additional systems,</p> $v = \begin{matrix} 13701.6 \\ 13403.4 \end{matrix} + 365(v' + \frac{1}{2}) - 3.95(v' + \frac{1}{2})^2 - 317(v'' + \frac{1}{2}) + 1.68(v'' + \frac{1}{2})^2,$ $v = \begin{matrix} 12697.6 \\ 12365.8 \end{matrix} + 365(v' + \frac{1}{2}) - 3.95(v' + \frac{1}{2})^2 - 354(v'' + \frac{1}{2}) + 3.00(v'' + \frac{1}{2})^2,$ <p>obtained under the same conditions at which the $d \rightarrow c$ bands of As_2 appear. Since they thought the latter were due to As_2^+ and since one of the new systems apparently has the same lower state (c) they concluded that both new systems belong to As_2^+. This conclusion is now very doubtful.</p>										
$^{75}\text{As}_2^-$										JAN 1976
I.P. = $0.1_0 \pm 0.1_8$ eV ^a										
$^{75}\text{As}^{(79)}\text{Br}$										JAN 1976
b (0^+)										
X	0									
(μ = 38.434024 ₅)										
0-0 sequence only; $\omega' - \omega'' = 15.0$ cm ⁻¹ .								b → X, V 12316.9 H	(1)*	
$^{75}\text{As}^{(35)}\text{Cl}$										JAN 1976
B	40826									
X	0	[520] H								
(μ = 23.8412199)										
443 H 2								B ← X, V 40865 H	(1)	

- As₂⁺: (1) Herzberg, MOLSPEC Vol. 1 (1950).
(2) Rao, Lakshman, IJPAP 4, 259 (1966).
- As₂⁻: ^aElectron impact mass-spectrometry (1).
(1) Bennett, Margrave, Franklin, Hudson, JCP 59, 5814 (1973).
- AsBr: (1) de Bie - Prévot, Thèse (Université Libre de Bruxelles,
1974)
- AsCl: (1) Basco, Yee, CC (1967), p. 1255.

State	T_e	w_e		$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
									Design.	ν_{00}	
$^{75}\text{As}^{19}\text{F}$		$\mu = 15.1553535$			$D_0^0 = 4.2 \text{ eV}^a$		$\text{I.P.} = 9.4 \text{ eV}^a$				JAN 1976 A
d 1_{Π}					$[0.3989]^b$		$[4.3]$	$[1.669_8]$	d \rightarrow b, V 37032.07 Z		(3)(5)
									d \leftrightarrow a, V 43628.60 Z		(3)(5)*
c (3_{Π})									d $\leftarrow X_1$, V 50686.43 Z		(6)
c 1_{Π}	48672.5	817.30	Z	4.39	0.4004 ^{cd}	0.0027	4.0	1.666 ₇	C \rightarrow X, V 49758 H		(6)
									c \rightarrow b, V 35083.56 Z		(3)(5)* (6)
									c \leftrightarrow a, V 41680.09 Z		(3)* (5)*
									c $\leftrightarrow X_2$, V 48599 ^e		(6)
									X_1 , 48737.92 Z		(6)*
B (3_{Π})	(48138)	815.5 ^f	H	3.9 ₆	Very complicated rotational structure.				B \leftrightarrow X, V 48202.2 ^f H		(6)*
c' 1_{Π}	32479.5	399.38	Z	1.34 ^g	0.2932 ^h	0.0018	6.2	1.948	c' \rightarrow b, R 18682.4		(7)*
									c' \rightarrow a, R 25278.88 Z		(7)*
									c' $\rightarrow X_2$, R 32198		(7)
Fragments of a system											
A ₄	$3_{\Pi r} \begin{cases} 2 & 27152 \\ 1 & 26348 \\ 0^+ & 25751 \\ 0^- & 25719 \end{cases}$	412.28	Z	1.43 ⁱ	0.2918	0.0020	6	1.954	A ₄ \rightarrow X ₂ , R 26877.0 Z		(10)*
A ₃		412.13	Z	1.44 ^j	0.2920 ^k	0.0020			A ₃ \rightarrow X ₁ , R 26211.7 Z		(10)*
A ₂		(419.8)	H		(0.2914)	(0.0018)			A ₂ \rightarrow X ₂ , R 25480		(10)
A ₁		412.21	Z	1.32 ^j	0.2904	0.0018			A ₁ \rightarrow X ₂ , R 25444.5 Z		(10)*
b 1_{Σ^+}	13648.6	697.34	Z	3.08	0.3719	0.0028	4.7	1.729 ₄	b $\rightarrow X_2$, ^l 13515.78 Z		(6)*
									X_1 , 13654.4 Z		(6)
a 1_{Δ}	7053.5	694.44	Z	3.06	0.3707	0.0026	4.4	1.732 ₂			
X ₂	$3_{\Sigma^-} \begin{cases} 1 & 138.7 \\ 0^+ & 0 \end{cases}$	685.50	H ^q	2.95	0.3691 ^{mn}	0.0028	4.5	1.736 ₀ ^m			
X ₁		685.78	Z	3.12	0.3648 ^{on}	0.0024					

AsF: ^aTheoretical calculations, for D_0^0 supported by limited experimental data; see (8). The same paper gives theoretical values for the electron affinity (1.1 eV) and dipole moment (1.75 D) of AsF.

^bPredissociated near $J=30$.

^c Λ -type doubling, $\Delta v_{ef} \approx + 0.00005 \times J(J+1)$.

^dPredissociation in $v=1$ at $J \approx 60$; $v=2$ observed in absorption only.

^eVery weak band.

^fThe vibrational analysis of (6) assigns $v=0$ to the lowest level observed in emission. However, the 1-0 and 0-0 bands may have been observed in absorption (4) at 49001 and 48192 cm^{-1} [47192 in (4) seems to be a misprint] as members of a strong upper state progression which begins at 47381 cm^{-1} and may even include a diffuse band at 46570 cm^{-1} . No details.

^g $w_e y_e = - 0.015$.

^h Λ -type doubling, $\Delta v_{ef} \approx + 0.000015 \times J(J+1)$.

ⁱ $w_e y_e = - 0.031$.

^j $w_e y_e = - 0.026$.

^kSmall Λ -type doubling.

^lLong 0-0 sequence of V shaded Q heads; R, P branches undegraded.

^m B_e and r_e from the f component; $\Delta v_{ef} = + 0.0035 \times J(J+1)$.

ⁿFor a more detailed discussion of the $X^3\Sigma^-(0^+, 1)$ fine structure see (9).

^oEffective value.

- (1) Pannetier, Deschamps, Guillaume, CR 261, 3396 (1965).
- (2) Pannetier, Deschamps, Guillaume, CR C 265, 710, (1967).
- (3) Yee, Liu, Jones, JMS 35, 153 (1970).
- (4) Chatalic, Danon, Pannetier, CR C 273, 874 (1971).
- (5) Liu, Yee, Jones, JMS 38, 512 (1971).
- (6) Liu, Jones, CJP 50, 1230 (1972).
- (7) Chatalic, Danon, Iacocca, Pannetier, JCPPB 70, 1600 (1973).
- (8) O'Hare, Batana, Wahl, JCP 59, 6495 (1973).
- (9) Veseth, JP B 6, 1473, 1484 (1973).
- (10) Chatalic, Danon, Pannetier, JCPPB 71, 243 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{75}\text{As}^1\text{H}$										
A $^3\Pi_1$	0	b	$\mu = 0.99444817$ [1207.5] ^c Z	$D_0^0 < 3.6 \text{ eV}^a$ [6.5623] ^{df} [6.4726] ^{ef} [6.3387] ^f	0.886 ^c	[70.3] [62.4] [55.4]	[1.6203] ^g	A \leftarrow X, R	30518.34 Z	FEB 1976 (1)* (2)
	1								29821.97 Z	
	2								29282.16 Z	
X $^3\Sigma^-$	0 ^h		(2130)	[7.1998] ^h		[32.9]	[1.5344]			
$^{75}\text{As}^2\text{H}$										
A $^3\Pi_1$	0	j	$\mu = 1.96137497$ [933.6] Z	$D_0^0 = 2.76 \text{ eV}^i$ [3.3467] ^{kf} [3.3220] ^{lf} [3.2881] ^f	0.264 0.240 0.227	[16.7] [16.1] [14.5]	[1.6095] ^g	A \leftarrow X, R	30628.87 Z	FEB 1976 (1)* (2)
	1								29932.48 Z	
	2								29389.55 Z	
X $^3\Sigma^-$	0 ^m		(1484)	[3.6688] ^m		[8.97] ⁿ	[1.5306]			(3)
$^{75}\text{As}^1\text{N}$										
A $^1\Pi$	35999.7		$\mu = 11.7979936_0$ [853.3] ^a Z 8.24 H	0.501 ₈ ^{bc}	0.009	0.066	1.687	A \rightarrow X, R	35899.6 Z	FEB 1976 A (1)* (5)* (6) (3)*
	($^1\Sigma^+$)								Single band.	
X $^1\Sigma^+$	0		1068.54 Z 5.41 ^d	0.54551 ^c	0.003366	0.053	1.6184 ₃			

As¹H, As²H:

^aFrom the predissociation in A ³Π.

^bA₀ = - 615.4. Small J-dependence (2).

^cΔG($\frac{1}{2}$) and α for the ³Π₀+ component only.

^dΛ-type doubling, Δv_{ef}(v=0) = + 44.72 + 0.0056 x J(J+1).

^eΛ-type doubling, Δv_{ef}(v=0) = + 0.0214 x J(J+1).

^fLines are sharp for the ³Π₀+ state only. Line width increases in the order ³Π₀+ < ³Π₀- < ³Π₁ < ³Π₂, and also with increasing vibrational energy. The predissociation is due to interaction with the unstable ⁵Σ⁻ state arising from As(⁴S) + H(²S) (1).

^gFrom the "true" B₀ values in (2).

^hSpin splitting constants λ₀ = + 58.87, γ₀ = - 0.281.

ⁱFrom a short extrapolation (1) of the ³Π state to the limit As(²D) + H(²S).

^jA₀ = - 616.9, small J-dependence (2); A₁ = - 599.8.

^kΛ-type doubling, Δv_{ef}(v=0) = + 43.39 + 0.00472 x J(J+1).

^lΛ-type doubling, Δv_{ef}(v=0) = + 0.0046 x J(J+1).

^mSpin splitting constants λ₀ = + 58.811, γ₀ = - 0.147₅.

ⁿH₀ = + 5 x 10⁻⁹.

(1) Dixon, Lamberton, JMS 25, 12 (1968).

(2) Veseth, JP B 5, 229 (1972).

(3) Lindgren, PS 12, 164 (1975).

AsN: ^aω_e = 871.3 from band heads (1).

^bStrong perturbations.

^cIndependent rotational analyses by (2) and (4) gave different B values. The values of (6) are based on plates with higher resolution and are adopted here.

^dω_ey_e = + 0.04.

(1) Spinks, ZP 88, 511 (1934).

(2) D'Incan, Fémelat, CR B 264, 1261 (1967).

(3) D'Incan, Fémelat, CR B 267, 796 (1968).

(4) Dixit, Krishnamurty, Narasimham, PIAS A 71, 23 (1970).

(5) Jones, JMS 34, 320 (1970).

(6) Fémelat, Jones, JMS 42, 388 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{75}\text{As}^{16}\text{O}$										
		$\mu = 13.1809344_6$		$D_0^0 \leq 4.980 \text{ eV}^a$						FEB 1976
B $2\Sigma^+$	39866.0	1098.3	H ^q 6.1	[0.51284] ^{bc}	0.0036 ^d	[4.57]	1.5764	B \leftrightarrow X, V	38905.88 Z 39931.36 Z	(1)(2)* (6)* (8)(14)
C $2\Delta_{5/2}$	38686 (38638)	655.7 ^e Only $v=0$ observed.	4.53	0.4164 ^e [0.4028]	0.0040	[14.1]	1.765	C \rightarrow X, R	37506 ^e 38483	(3)(15)(17)
C' 2ϕ or 2Δ	(38800)	(600) ^f		(0.3798) ^f	(0.0058)					(15)(17)
D $2\Sigma^-$	37555.4	629.9 ^g	Z 3.79	0.3973 ^{gh}	0.0034	6.5	1.794 ₂	D \rightarrow X, R	36361.7 Z 37387.1 Z	(3)(6)(7)(8) (11)(13)(15) (17)
D' $2\Sigma^-$	[37857] ⁱ			[0.360] ⁱ						(17)
H $2\Pi_{1/2}$	37053.7	606.92	Z 4.913	0.36539 ^{kl}	0.00273	5.4	1.8709	H \rightarrow X, R	35848.2 Z	(12)(17)
A $2\Sigma^+$	31652.45	686.68	Z 10.78	0.46240 ^{mn}	0.00710	8.56 ^o	1.6631	A \rightarrow X, R	30485.28 Z 31510.87 Z	(1)* (2)* (4)(6)* (8) (14)
Fragments of additional systems of R shaded emission bands in the region 25000 - 30000 cm^{-1} .										
A' $2\Pi_i$	26485.2 ^p 26168.4	630.30 Z 633.23 Z	3.006 ^r 2.895	0.37183 ^{ksp} 0.37124 ^k	0.002701 0.002622	5.0	1.8553	A' \rightarrow X, R	26317.30 Z 24976.59 Z	(6)(10)* (11)(16)(17)
Fragments of a weak system of R shaded emission bands in the region 15300 - 17300 cm^{-1} .										
X $2\Pi_r$	1025.97 ^t 0	965.90 Z 967.08 Z	4.909 ^u 4.850 ^v	0.48552 ^k 0.48482 ^{kw}	0.003320 ^u 0.003299 ^v	4.9	1.6236			(16)
$^{75}\text{As}^{16}\text{O}^+$										
A 1Π	42594.2	780.8	Z 7.4	0.4491 ^a	0.0047	5.0	1.688	A \rightarrow X, R	42433.4 Z	(1)(2)(4)* (5)
X $1\Sigma^+$	0	[1091.32]	Z 5.0 H	0.5199 ^a	0.0031	3.9	1.568			

AsO: ^aFrom the predissociation in B $^2\Sigma^+$.
^bSpin splitting constant $\gamma_0 = +0.0043$.
^cWeak predissociation above $v=0, N=20$ (23 for As ^{18}O) (6) (8), attributed (6) to interaction with the unstable $^4\Sigma^+$ state arising from ground state atomic products.
^dEstimated from band head separations.
^eDeperturbed (15) constants. Strong perturbations by successive levels in both doublet components of a $^2\phi$ or $^2\Delta$ state, and possibly by other states.
^fFrom perturbations in C $^2\Delta_{5/2}$. Vibrational numbering unknown.
^g $v=0$ and 1, formerly (12) attributed to a $^4\Sigma$ state, are perturbed by levels of a $^2\Sigma^-$ state and of H $^2\Pi_{\frac{1}{2}, \frac{1}{2}}$ (17).
^hThe spin splitting constant γ_v increases from $\gamma_0 = +0.021$ to $\gamma_7 = +0.039$.
ⁱLowest observed level, from a perturbation in D ($v=0$). Vibrational numbering unknown.
^jBands of the $\frac{1}{2} - \frac{1}{2}$ transition have not been identified. One level of $^2\Pi_{\frac{1}{2}}$ (vibrational numbering unknown) may be responsible for a perturbation in D $^2\Sigma^-(v=0)$.
^kEffective constants.
^lPerturbations in $v=1, 2$ by $v=0, 1$, resp., of D $^2\Sigma^-$.
^mSpin splitting constant $\gamma = -0.035$.
ⁿ $v=0, 1, 2$ perturbed by $v=9 \dots 12$ of A' $^2\Pi_{\frac{1}{2}}$. Additional perturbations by unidentified levels of Σ and Π symmetry (6)(17).
^o $\beta_e = +0.18 \times 10^{-7}$; $H_e = -2.6 \times 10^{-12}$.
^pThe levels $v=9 \dots 12$ of $^2\Pi_{\frac{1}{2}}$ have been observed in perturbations of A $^2\Sigma^+(v=0, 1, 2)$ and were previously (6) assigned to a state G $^2\Pi$.
^q $A_e = -316.08$.
^r $w_e y_e = +0.010$.

AsO (continued):

^s Λ -type doubling $\Delta v_{fe} = -0.002(J + \frac{1}{2})$.
^t $A_e = +1026.94$.
^u $w_e y_e = -0.0034$; $\gamma_e = -4.6 \times 10^{-6}$.
^v $w_e y_e = -0.0015$; $\gamma_e = -2.5 \times 10^{-6}$.
^w Λ -type doubling $\Delta v_{fe} = +0.0179(J + \frac{1}{2})$.

- (1) Connelly, PPS 46, 790 (1934).
- (2) Jenkins, Strait, PR 47, 136 (1935).
- (3) Lakshman, Rao, IJP 34, 278 (1960).
- (4) Klynning, Naturw. 49, 252 (1962).
- (5) Venkataramanaiah, Lakshman, IJP 38, 209 (1964).
- (6) Callomon, Morgan, PPS 86, 1091 (1965).
- (7) d'Incan, Goure, CR 261, 3086 (1965).
- (8) Meyer, JMS 18, 443 (1965).
- (9) d'Incan, Goure, Zgainsky, CR B 263, 1319 (1966).
- (10) Mrozowski, Santaram, JOSA 56, 1174 (1966).
- (11) Goure, d'Incan, CR B 268, 1311 (1969).
- (12) d'Incan, Goure, CR B 268, 1647 (1969).
- (13) Topouzkhaniyan, Goure, Figuet, d'Incan, CR B 270, 1676 (1970).
- (14) Lakshman, Rao, JP B 4, 269 (1971). | (1970).
- (15) Goure, Figuet, Massot, d'Incan, CJP 50, 1926 (1972).
- (16) Kushawaha, Asthana, Pathak, JMS 41, 577 (1972).
- (17) Anderson, Callomon, JP B 6, 1664 (1973).

AsO $^+$: ^aDifferent constants in (3).

- (1) See ref. (3) of AsO.
- (2) Lakshman, PPS 89, 774 (1966).
- (3) Shanker, Singh, Singh, CJP 47, 1601 (1969).
- (4) Rao, Rao, JP B 3, 430 (1970).
- (5) See ref. (14) of AsO.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{75}\text{As}^{31}\text{P}$		$\mu = 21.9141220$								FEB 1976
A $^1\Pi$	32417.05	475.52	Z 2.12	0.1744 ^a	0.0009	11	2.100	A \rightarrow X, R	32352.76 Z	(1)(2)*
X $^1\Sigma^+$	0	604.02	Z 1.98	0.1925	0.0008	7.8	1.999			
$^{75}\text{As}^{32}\text{S}$		$\mu = 22.4091734$								FEB 1976 A
		Unclassified bands, most of them red-degraded, in the region 26000 - 31000 cm^{-1} .								(1)
A ₂ $^2\Pi_{1/2}$	20474.9	[399.84]	Z	0.14871 ^a	0.00073	8.1 ^b	2.2496	A ₂ \rightarrow X ₁ , R	20392.13 Z	(4)*
A ₁ $^2\Pi_{3/2}$	x + 19263.28	405.58	Z 1.11	0.14859	0.00069 ^c	8.0 ^b		A ₁ \rightarrow X ₂ , R	19183.22 Z	(2)* (3)* (5)*
X ₂ $^2\Pi_{3/2}$	x	566.13	Z 1.96 ^d	0.18492	0.00083	7.9 ^b	2.0174			
X ₁ $^2\Pi_{1/2}$	0	567.94	Z 1.97	0.18476 ^a	0.00082	7.8 ^b				
$^{75}\text{As}^{32}\text{S}^+$										FEB 1976
A $^1\Pi$	37359.7	441.18	Z 3.45	0.1732 ^a	0.00123	10.0	2.084	A \rightarrow X, R	37257.82 Z	(1)(2)*
X $^1\Sigma^+$	0	644.25	Z 2.09	0.1989	0.00089	5.7	1.9447			
$^{75}\text{As}^{(80)}\text{Se}$		$(\mu = 38.669248_6)$								FEB 1976
A ($^2\Pi$)								A \rightarrow X, R	18717 H 18044 H	(1)
X ($^2\Pi$)	0	281	H 0.5							

AsP: ^aSmall perturbations in both Λ -components [see (2)].

(1) Yee, Jones, CC (1969), p. 586.

(2) Harding, Jones, Yee, CJP 48, 2842 (1970).

AsS: ^a Λ -type splitting in the $2\Pi_{\frac{1}{2}} - 2\Pi_{\frac{1}{2}}$ subbands $\Delta v \approx 0.037(J + \frac{1}{2})$.

^bValues of $4B_e^3/\omega_e^2$, in satisfactory agreement with experimental values.

^c $\gamma_e = +5 \times 10^{-6}$.

^d $\omega_e v_e = -0.003_1$.

(1) Shimauchi, SL 18, 90 (1969).

(2) Shimauchi, CJP 49, 1249 (1971).

(3) Shimauchi, Sakaba, Kikuchi, SL 21, 1 (1972).

(4) Shimauchi, Iwata, Matsuno, Sakaba, Lee, Karasawa, SL 21, 145 (1972).

(5) Shimauchi, Karasawa, SL 22, 127 (1973).

AsS⁺: ^aSmall perturbations in both Λ -components [see (2)].

(1) See ref. (1) of AsS.

(2) Shimauchi, Karasawa, Ninomiya, SL 23, 72 (1974); Shimauchi, Karasawa, CJP 53, 831 (1975).

AsSe: (1) Vasudev, Jones, JMS 54, 144 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{197}\text{Au}_2$		$\mu = 98.483274$ $D_0^0 = 2.30 \text{ eV}^a$								FEB 1975
B	0_u^+ 25685.5	179.85	H	0.680 ^b	[0.026961]	(0.0000963)	[0.260]	[2.5197]	B \leftrightarrow X, R 25679.87 Z	(2)(5)* (8)*
A	0_u^+ 19668.1	142.3	H	0.445 ^c	0.02595 ₈	0.0000903	0.35	2.567 ₉	A \leftrightarrow X, R 19643.8 H	(1)* (2)(5) (8)
X	1_{Σ}^+ _g 0	190.9 ^d	H	0.420 ^e	0.028013 ^f	0.0000723	[0.250]	2.4719		
$^{197}\text{Au}^{27}\text{Al}$		$\mu = 23.7307715$ $D_0^0 = 3.34 \text{ eV}^a$								NOV 1974
C	1 24623	250	H	2	[0.12332 ₂] ^b		[11.5 ₉]	[2.4001]	C \leftrightarrow X, R 24581.28 Z	(1)(2)*
B	1 22490.3	291.83	H ^Q	3.03	0.13131 ^c	0.00130	(10.5)	2.3259	B \leftrightarrow X, R ^d 22469.22 H ^Q	(1)(2)*
A	0^+ 16265.06	347.96	Z	1.85 ₄	0.13645 ₅	0.00084 ₈	7.80 ^e	2.2816 ₄	A \leftrightarrow X, V 16272.37 Z	(1)(2)* (3)
X	1_{Σ}^+ (0^+) 0	333.00	Z	1.16 ₃	0.12991 ₃	0.00066 ₈	7.18 ^f	2.3383 ₉		
$^{197}\text{Au}^{75}\text{As}$		$\mu = 54.276176_0$								NOV 1974
System D:		$v_H = 18471.2 + 228.1(v' + \frac{1}{2}) - 0.8(v' + \frac{1}{2})^2 - 254.8(v'' + \frac{1}{2}) + 0.6(v'' + \frac{1}{2})^2$						a	R 18457.8 H	(1)
System C:		$v_H = 17442.1 + 242.2(v' + \frac{1}{2}) - 1.1(v' + \frac{1}{2})^2 - 257.7(v'' + \frac{1}{2}) + 0.8(v'' + \frac{1}{2})^2$						a	R 17434.3 H	(1)
System B:		$v_H = 16582.1 + 241.7(v' + \frac{1}{2}) - 0.9(v' + \frac{1}{2})^2 - 254.8(v'' + \frac{1}{2}) + 0.6(v'' + \frac{1}{2})^2$						a	R 16575.5 H	(1)
System A:		$v_H = 16473.5 + 226.9(v' + \frac{1}{2}) - 1.1(v' + \frac{1}{2})^2 - 239.3(v'' + \frac{1}{2}) + 0.7(v'' + \frac{1}{2})^2$						a	R 16467.2 H	(1)
$^{197}\text{Au}^{(11)}\text{B}$		$(\mu = 10.4265222_7)$ $D_0^0 = 3.6_5 \text{ eV}^a$								NOV 1974
$^{197}\text{Au}^{(138)}\text{Ba}$		$(\mu = 81.113786)$								NOV 1974
		Unclassified R shaded bands in the region 13500 - 14100 cm^{-1} ; assignment to AuBa uncertain. ^a								(2)
B	21804	137.5	H	0.5 ^b				B \rightarrow (X), ^a v_R	21808 H	(1)(2)
A'	13522	154.1	H	0.35				A' \rightarrow (X), ^{ac} V	13535 H	(2)
A	12636.4	158.1	H	0.30				A \rightarrow X, ^a V	12651.0 H	(1)(2)
X	0	128.8	H	0.18						

Au₂:
^aThermochemical value (mass-spectrom.)(3)(4)(6), recalculated (9)(10), and (11).
^b $w_e v_e = +0.003$.
^c $w_e v_e = -0.0015$.
^dFrom band origins $\Delta G(\frac{1}{2}) = 190.176$ (8).
^e $w_e v_e = -0.0001$.
^fGround state potential curve (7).
 (1) Kleman, Lindkvist, Selin, AF 8, 505 (1954).
 (2) Ruamps, CR 238, 1489 (1954).
 (3) Drowart, Honig, JCP 25, 581 (1956); JCP 61, 980 (1957).
 (4) Schissel, JCP 26, 1276 (1957).
 (5) Ruamps, AP(Paris) 4, 1111 (1959).
 (6) Ackerman, Stafford, Drowart, JCP 33, 1784 (1960).
 (7) Dolgushin, OS(Engl. Transl.) 19, 289 (1965).
 (8) Ames, Barrow, TFS 63, 39 (1967).
 (9) Smoes, Drowart, CC (1968), p. 534.
 (10) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).
 (11) Kordis, Gingerich, Seyse, JCP 61, 5114 (1974).

AuAl:
^aThermochemical value (mass-spectrom.)(4).
^bAverage of the two Ω -type doubling components;
 $\Delta v_{fe} = +0.00011 J(J+1)$.
^cFrom bandhead measurements, using ground state constants from A-X.
^dReversal of shading in the 0-0 band from V at low J to R at high J.

AuAl (continued):

$$^e\beta_e = +0.06 \times 10^{-8}.$$

$$^f\beta_e = -0.01 \times 10^{-8}.$$

- (1) See ref. (5) of Au₂.
- (2) Barrow, Travis, PRS A 273, 133 (1963).
- (3) Lochet, CR B 272, 797 (1971).
- (4) Gingerich, Blue, JCP 59, 185 (1973).

AuAs: ^aThermal emission and absorption.

- (1) Houdart, Bocquet, CR B 264, 1717 (1967).

AuB: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1) Gingerich, ZN 24 a, 293 (1969); JCP 54, 2646 (1971).
- (2) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart, TFS 66, 809 (1970).

AuBa: ^aAll systems in thermal emission.

^bAnalysis uncertain.

^cIt is assumed that the lower state of this system ($w_e'' = 128.8$, $w_e'' x_e'' = 0.44$) is identical with the lower state of A-X.

- (1) Schiltz, CR 253, 1777 (1961).
- (2) Schiltz, AP(Paris) 8, 67 (1963).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{197}\text{Au}^9\text{Be}$		$\mu = 8.6178730$								NOV 1974
B $\frac{1}{2} ({}^2\Pi_{\frac{1}{2}})$	18945.98	628.9 ₅	Z^a 3.22 ₅ ^b	0.47944 ^c	0.00434	[1.09] ^d	2.0199 ₁	B \leftrightarrow X, V	18956.68 Z	(1)* (2)
A $\frac{1}{2} ({}^2\Sigma^+)$	17171.04	655.4 ₄	Z^a 3.59 ₅	0.49264 ^f	0.00463	[1.09] ^g	1.9926 ₆	A \leftrightarrow X, V	17194.88 Z	(1)* (2)
X ${}^2\Sigma^+$	0	607.68	Z^a 3.53	0.46074	0.00400	[1.04] ^h	2.0604 ₉			(1)(2)
$^{197}\text{Au}^{209}\text{Bi}$		$\mu = 101.397851$								NOV 1974
A	17787.4	149.6	H ^a 0.34					A \leftarrow X, R	17783.3 H	(1)*
X	0	157.7	H ^a 0.25							
$^{197}\text{Au}^{(40)}\text{Ca}$		$(\mu = 33.2221432)$								NOV 1974 A
		Very complex system of R and V shaded bands in the region 16000 - 19000 cm^{-1} . ^a								(1)*
B	15024.8	220.2	H ^Q 0.6					B \rightarrow (X) ^{b, a} V	15024.1 H ^Q	(1)*
A	14512.3	212.7	H ^Q 0.10					A \rightarrow X, ^a V	14508.8 H ^Q	(1)
X	0	220.0	H ^Q 0.62 ^c							
$^{197}\text{Au}^{(140)}\text{Ce}$		$(\mu = 81.801686) \quad D_0^0 = 3.3_4 \text{ eV}^a$								NOV 1974
$^{197}\text{Au}^{35}\text{Cl}$		$\mu = 29.6966066 \quad D_0^0 = (3.5) \text{ eV}$								NOV 1974
B	19238.3	316.3	H 1.45					B \rightarrow X, R	19205.0 H	(1)*
A	19113.8	312.0	H 0.70					A \rightarrow X, R	19078.6 H	(1)*
X (${}^1\Sigma^+$)	0	382.8	H 1.30							
$^{197}\text{Au}^{59}\text{Co}$		$\mu = 45.360994_8 \quad D_0^0 = 2.2_2 \text{ eV}^a$								NOV 1974

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{197}\text{Au}^{(52)}\text{Cr}$		$(u = 41.101859_8) \quad D_0^0 = 2.2_5 \text{ eV}^a$								NOV 1974

AuBe: ^aUsing calculated head-origin separations.

$$^b w_e v_e = -0.065_8.$$

^cAverage of the two Ω -type doubling components;

$$\Delta v_{\text{Fe}}(v=0) = -0.0189_5(J+\frac{1}{2}) + \dots$$

$$^d H_0 = -8.1 \times 10^{-13}.$$

$$^e w_e v_e = -0.19_3.$$

^fAverage of the two Ω -type doubling components;

$$\Delta v_{\text{Fe}}(v=0) = +0.1057_9(J+\frac{1}{2}) + \dots$$

$$^g H_0 = -11.1 \times 10^{-13}.$$

$$^h H_0 = -5.4 \times 10^{-13}.$$

(1) Barrow, Gissane, Travis, Nature 201, 603 (1964);
PRS A 287, 240 (1965).

(2) Singh, Pathak, JQSRT 10, 819 (1970).

AuBi: ^aFrom the variation of $\Delta G(v+\frac{1}{2})$ along the rows and columns of the Deslandres table it appears that the head-origin separations are very large.

(1) Houdart, Bocquet, CR B 263, 151 (1966).

AuCa: ^aThermal emission.

^bThe lower state of this transition ($w_e = 221.85$, $w_e x_e = 1.08$, $w_e v_e = +0.042$) is probably identical with the lower state of $A \rightarrow X$.

$$^c w_e v_e = +0.01.$$

(1) Schiltz, CR 252, 1750 (1961); AP(Paris) 8, 67 (1963).

AuCe: ^aThermochemical value (mass-spectrom.)(1).

(1) Gingerich, Finkbeiner, JCP 52, 2956 (1970); 54, 2621 (1971).

AuCl: (1) Ferguson, PR 31, 969 (1928).

AuCo: ^aThermochemical value (mass-spectrom.)(1)(2).

(1) Kant, JCP 40, 5144 (1968).

(2) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

AuCr: ^aThermochemical value (mass-spectrom.)(1).

(1) Ackerman, Stafford, Verhaegen, JCP 36, 1560 (1962).

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻⁴ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	ν ₀₀	
¹⁹⁷Au(⁶³)Cu										
		(μ = 47.692221 ₁) D ₀ ⁰ = 2.3 ₆ eV ^a Unclassified R shaded bands in the region 16900 - 19600 cm ⁻¹ .								NOV 1974
D	(23699)	(182)	H					D→X,	R (23665)	H (1)
C	(22176)	(231)	H					C→X,	R (22167)	H (1)
B	(20655)	(250) ^b	H					B→X,	R 20655.4	H (1)
A	(20241)	[195.7] ^c	H					A→X,	R 20214	H (1)
X	0	250	H	0.7						
¹⁹⁷Au¹⁹F ?										
		μ = 17.3271178 Stimulated IR emission in the range 420 - 950 cm ⁻¹ .								JAN 1975 (1)
¹⁹⁷Au(⁵⁶)Fe										
		(μ = 43.563646 ₈) D ₀ ⁰ = 1.9 ₀ eV ^a								NOV 1974
¹⁹⁷Au⁶⁹Ga										
		μ = 51.058425 ₈								NOV 1974
A	(0 ⁺) 18061.6	219.1	H	1.22 ^a		b		A↔X,	ν _R 18058.0	H (1)(2)(3)
X	(0 ⁺) 0	226.0	H	0.61		b				
¹⁹⁷Au(⁷⁴)Ge										
		(μ = 53.749202 ₉)								NOV 1974
A	(² Σ) 13743.3	242.6 ^a	H	0.59				A↔X ₂ ,	R ^b (12188)	H (1)(2)* (3)
X ₂	(² Π _{3/2}) (1552)							A↔X ₁ ,	R ^b 13739.7	H
X ₁	(² Π _{1/2}) 0	249.7 ^a	H	0.33						
¹⁹⁷Au¹H										
		μ = 1.00269470 D ₀ ⁰ = 3.2 ₂ eV ^a								NOV 1974
C	1Σ ⁺ (43350)	(1550) ^b				[(6.66)] ^b		C←X,	R (42986) ^b	(5)*
c	0 ⁻ 42922	[1229]	Z (42)		5.96	0.27	[5.3] ^c	c←X, ^d	R 42426	Z (5)
b	1 42883	[1075.9]	Z (58)		5.627 ^e	0.320	[3.5]	b←X, ^e	R 42323.0	Z (5)
a	2 (42720)	(1020)	(45)		[5.523] ^f	f	[3.9]	a←X,	R 42077.1	Z (5)

AuCu: ^aThermochemical value (mass-spectrom.)(2).
^bPerturbations.
^cPerturbations; irregular vibrational intervals.
 (1) Ruamps, CR 239, 1200 (1954); SA(Suppl.) 11, 329 (1957).
 (2) Ackerman, Stafford, Drowart, JCP 33, 1784 (1960).

AuF: (1) Rice, Beattie, CPL 19, 82 (1973).

AuFe: ^aThermochemical value (mass-spectrom.)(1).
 (1) Kant, JCP 49, 5144 (1968).

AuGa: ^a $w_{ey_e} = -0.0049$.
^bFor rotational constants derived from incompletely resolved rotational structure in the 0-0 band see (4). Uncertain.
 (1) Barrow, Gissane, Travis, Nature 201, 603 (1964).
 (2) Bocquet, Houdart, CR B 265, 979 (1967).
 (3) Locket, CR B 272, 797 (1971).
 (4) Bocquet, Lefebvre, Houdart, JP(Paris) 34, 317 (1973).

AuGe: ^aFrom (3). (1) give $\Delta G'(\frac{1}{2}) = 244$, $\Delta G''(\frac{1}{2}) = 251.7$ (from bandheads).
^bMultiple heads. No analysis of $A \leftrightarrow X_2$.
 (1) See ref. (1) of AuGa.
 (2) Houdart, CR 261, 2609 (1965).
 (3) Houdart, Schamps, JP B 6, 2478 (1973).

Au¹H, Au²H:

^aBased on the value for the common dissociation limit Au(²D_{3/2}) + H(²S) of states B, a, b, and c (5). Agrees within error limits with an earlier thermochemical value by (1).
^bApproximate constants for the deperturbed state. Perturbed values are $B_0 = 5.79$, $v_0(0-0) = 43105.5$. Rotational levels in $v=0$ are broadened; broadening increases with J. See ^j.
^c $D_1 = 7.6 \times 10^{-4}$.
^dQ branches only having $J \geq 18$.
^e Ω -type doubling $\Delta v_{ef}(v=0) \approx +0.006 J(J+1) + 0.00007 J^2(J+1)^2 - \dots$ for $J < 17$. b 1($v=0$) perturbed by B 0⁺($v=3$) at $J \approx 18$. Bands with $v' \geq 1$ consist of Q branches only.
^f Ω -type doubling $\Delta v_{ef}(v=0) \approx -0.005 J(J+1) + 0.00002 J^2(J+1)^2$. Bands ascribed by (5) to $v=4$ and 5 ($B_4 = 4.60$, $B_5 = 3.63$) consist of Q branches only; line width increasing with J, see ^j.

(continued p. 57)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{197}\text{Au}^1\text{H}$ (continued)										
B 0^+ ^8 (38545)		[1544.5]	Z (74) ^h	5.849 ^{ij}	0.187 ^h	[3.0] ^k	1.695 ₄	B \leftrightarrow X, R 38231.8	Z	(2)(5)* (6)
A 0^+ ^8 27665.7		1669.55	Z 55.06 ^l	6.0069	0.249 ^l	3.24 ^l	1.6729 ₇	A \leftrightarrow X, R 27344.5	Z	(1)(2)(3) (4)* (6)
X $1\Sigma^+$ 0		2305.01	Z 43.12 ^m	7.2401	0.2136	2.79 ^m	1.5238 ₅			
$^{197}\text{Au}^2\text{H}$										
C $1\Sigma^+$ (43350)		$\mu = 1.99371527$	$D_0^0 = 3.2_6 \text{ eV}^n$							NOV 1974
b 1 (42838)		(1100) ^o	$[(3.53)]^o$				$[(1.54_8)]^o$	C \leftarrow X, R (43086) ^o		(5)*
a 2		(845) ⁿ	(29) ⁿ	[2.762] ^p		[0.93]	[1.749 ₇]	b \leftarrow X, R 42440.7	Z	(5)
B 0^+ 38531.9		Identification uncertain.						a \leftarrow X, R		(5)
A 0^+ 27644.1		1187.4	Z 33.9 ^q	2.951 ^r	0.067 ^q	0.73 ^q	1.692 ₇	B \leftrightarrow X, R 38305.1	Z	(2)(5)*
X $1\Sigma^+$ 0		1195.24	Z 34.813	3.0352	0.0963 ^s	0.79 ^s	1.6690 ₆	A \rightarrow X, R 27420.9	Z	(2)(3)*
		1634.98	Z 21.655 ^t	3.6415	0.07614	0.709 ^t	1.5237 ₉			
$^{197}\text{Au}^{165}\text{Ho}$										
		$\mu = 89.765242$	$D_0^0 = 2.7 \text{ eV}^a$							FEB 1975
$^{197}\text{Au}^{(115)}\text{In}$										
		$(\mu = 72.569304)$								NOV 1974
		Red degraded bands in the region 15600 - 17900 cm^{-1} .								(1)
$^{197}\text{Au}^{139}\text{La}$										
		$\mu = 81.459119$	$D_0^0 = 3.4_5 \text{ eV}^a$							NOV 1974
$^{197}\text{Au}^{(7)}\text{Li}$										
		$(\mu = 6.7746885)$			$D_0^0 = 2.92 \text{ eV}^a$					APR 1975 A
$^{197}\text{Au}^{(175)}\text{Lu}$										
		$(\mu = 92.650724)$			$D_0^0 = 3.4_1 \text{ eV}^a$					NOV 1974
$^{197}\text{Au}^{(24)}\text{Mg}$										
		$(\mu = 21.3813864)$								NOV 1974
		Additional unidentified R shaded absorption bands in the region 38230 - 37580 cm^{-1} .								(2)

Au^1H , Au^2H (continued):

^gA and B correspond to $^1\Sigma^*$ and $^1\Sigma^{**}$, respectively, of (2).

^hVibrational levels observed up to $v=4$. Levels with $v \geq 2$ are strongly perturbed by C $^1\Sigma^+$. For details see (5).

ⁱBroadening, increasing with J, of rotational levels in $v=3$ and 4. See ^j.

^jPredissociations in $\text{B}0^+$, a2, and C $^1\Sigma^+$ are due to interaction with an unstable 1 state arising from $\text{Au}(^2\text{D}_{5/2}) + \text{H}(^2\text{S})$; see (5).

^k $D_1 = 3.4 \times 10^{-4}$.

^l $w_e y_e = -3.93$; $\gamma_e = -0.027$; $\beta_e = +0.28 \times 10^{-4}$.

^m $w_e y_e = -0.044$; $\beta_e = -0.0084 \times 10^{-4}$.

ⁿFrom the value for Au^1H .

^oApproximate constants for the deperturbed state. Perturbed values are $B_0 = 2.954$, $v_0(0-0) = 43011.0$. Constants for an additional level at 45122.8 cm^{-1} above X $^1\Sigma^+(v=0)$, assumed to be unperturbed and tentatively assigned as $v=2$, are $B_2 = 2.75$, $D_2 = 8.3 \times 10^{-4}$.

^pAverage of the two Ω -type doubling components;

$\Delta v_{\text{ef}} \approx +0.0055 J(J+1)$.

^qVibrational levels observed for $v \leq 7$, except $v=6$.

Levels with $v > 2$ are strongly perturbed by C $^1\Sigma^+$ (5).

$\beta_e \approx +0.06 \times 10^{-4}$.

^rLine width in $5 \leftarrow 0$ band increases with J.

^s $\gamma_e = -0.0038$; $\beta_e = +0.071 \times 10^{-4}$.

^t $w_e y_e = -0.0288$; $\beta_e = -0.0034 \times 10^{-4}$.

Au^1H , Au^2H (continued):

(1) Farkas, ZPC B 5, 467 (1929).

(2) Heimer, Naturw. 24, 78 (1936); ZP 101, 121 (1936); 104, 303 (1937); Dissertation (Stockholm, 1937).

(3) Imanishi, Sci. Pap. IPCR (Tokyo) 31, 247 (1937).

(4) Nilsson, Dissertation (Stockholm, 1948).

(5) Ringström, Nature 198, 981 (1963); AF 27, 227 (1964).

(6) Loginov, OS (Engl. Transl.) 16, 220 (1964).

AuHo: ^aThermochemical value (mass-spectrom.)(1)(2)(3).

(1) Cocke, Gingerich, JPC 75, 3264 (1971).

(2) Gingerich, CPL 13, 262 (1972).

(3) Kordis, Gingerich, Seyse, JCP 61, 5114 (1974).

AuIn: (1) Barrow, Gissane, Travis, Nature 201, 603 (1964).

AuLa: ^aThermochemical value (mass-spectrom.)(1).

(1) Gingerich, Finkbeiner, JCP 52, 2956 (1970); 54, 2621 (1971).

AuLi: ^aThermochemical value (mass-spectrom.)(1).

(1) Neubert, Zmbov, JCS FT I 70, 2219 (1974).

AuLu: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (2) of AuHo.

AuMg: See p. 59.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{197}\text{Au}^{(2+)}\text{Mg}$ (continued)										
D		Six R shaded bands in the region 34230 - 32720 cm^{-1} . No analysis.						D \leftarrow X, R	(2)	
C	31058	242	H	2^a				C \leftarrow X, R 31025 H	(2)	
B $\frac{1}{2}$ ($^2\Pi_{\frac{1}{2}}$)	19492.3	338.5	H ^Q	1.46^b	$[0.14043]^c$	$[1.02]^d$	$[2.3695]$	B \leftrightarrow X, V 19507.52 Z	(1)(3)	
A $\frac{1}{2}$ ($^2\Sigma^+$)	18392.7	341.7	H	3.3	$[0.14201]^e$	$[1.06]^f$	$[2.3562]$	A \leftrightarrow X, V 18409.05 Z	(1)* (3)	
X $2\Sigma^+$	0	307.9 ^g	H	1.1	0.13214	0.00073	$[1.02]^h$ 2.4427			
$^{197}\text{Au}^{55}\text{Mn}$		$\mu = 42.956570_0$ $D_0^0 = 1.8_8 \text{ eV}^a$							NOV 1974	
$^{197}\text{Au}^{(142)}\text{Nd}$		$(\mu = 82.482152)$ $D_0^0 = 3.0_6 \text{ eV}^a$							NOV 1974	
$^{197}\text{Au}^{(58)}\text{Ni}$		$(\mu = 44.767511_8)$ $D_0^0 = 2.5_3 \text{ eV}^a$							NOV 1974	
$^{197}\text{Au}^{16}\text{O}$		$\mu = 14.7935835_5$ $D_0^0 = 2.3_3 \text{ eV}^a$							NOV 1974 A	
$^{197}\text{Au}^{(208)}\text{Pb}$		$(\mu = 101.160962)$ A second system under low resolution near 8800 cm^{-1} , possibly due to A \rightarrow X ₂ . ^a							NOV 1974	
A	16357.6	152.7	H	0.9				A \rightarrow X ₁ . ^a R 16354.6 H	(2)	
X ₁	0	158.6	H	0.6					(1)*	
$^{197}\text{Au}^{(106)}\text{Pd}$		$(\mu = 68.872592)$ $D_0^0 = 1.4_4 \text{ eV}^a$							NOV 1974	
$^{197}\text{Au}^{141}\text{Pr}$		$\mu = 82.143292$ $D_0^0 = 3.1_2 \text{ eV}^a$							NOV 1974	
$^{197}\text{Au}^{(32)}\text{S}$		$(\mu = 27.5070619)$ $D_0^0 = 2.5_9 \text{ eV}^a$							NOV 1974	

AuMg: ^a $w_e y_e = -0.1$.
^b $w_e y_e = +0.009$.
^cAverage of the two Ω -type doubling components;
 $\Delta v_{fe}(v=0) = -0.0039_3(J+\frac{1}{2}) + \dots$
^d $H_0 = +1.54 \times 10^{-13}$.
^eAverage of the two Ω -type doubling components;
 $\Delta v_{fe}(v=0) = +0.0264_0(J+\frac{1}{2}) + \dots$
^f $H_0 = +0.96 \times 10^{-13}$.
^gFrom band origins $\Delta G(\frac{1}{2}) = 306.10$.
^h $H_0 = +1.56 \times 10^{-13}$.
 (1) Ruamps, AP(Paris) 4, 1111 (1959).
 (2) Schiltz, CR 251, 682 (1960).
 (3) Barrow, Gissane, Travis, Nature 201, 603 (1964);
 PRS A 287, 240 (1965).

AuMn: ^aThermochemical value (mass-spectrom.)(1).
 (1) Smoes, Drowart, CC (1968), 534.

AuNd: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, Finkbeiner, JCP 52, 2956 (1970);
54, 2621 (1971).

AuNi: ^aThermochemical value (mass-spectrom.)(1)(2).
 (1) Kant, JCP 42, 5144 (1968).
 (2) Smoes, Mandy, Vander Auwera-Mahieu, Drowart,
 BSCB 81, 45 (1972).

AuO: ^aThermochemical value (mass-spectrom.)(1).
 (1) See ref. (2) of AuNi.

AuPb: ^aThermal emission.
 (1) Houdart, Carette, CR 260, 5746 (1965).
 (2) Houdart, Schamps, JP B 6, 2478 (1973).

AuPd: ^aThermochemical value (mass-spectrom.)(1).
 (1) Ackerman, Stafford, Verhaegen, JCP 36, 1560
 (1962).

AuPr: ^aThermochemical value (mass-spectrom.)(1).
 (1) See ref. (1) of AuNd.

AuS: ^aThermochemical value (mass-spectrom.)(2). See,
 however, (1) who gives $D_0^0 = 4.2_4$ eV.
 (1) Gingerich, CC (1970), 580.
 (2) See ref. (2) of AuNi.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{197}\text{Au}^{(121)}\text{Sb}$		$(\mu = 74.917358_6)$ Four systems of R shaded bands, presumably in thermal emission: System D: $\nu_H = 16762.3 + 186.2(\nu' + \frac{1}{2}) - 0.6(\nu' + \frac{1}{2})^2 - 203(\nu'' + \frac{1}{2}) + 0.4(\nu'' + \frac{1}{2})^2$. System C: $\nu_H = 16108.6 + 192.8(\nu' + \frac{1}{2}) - 0.3(\nu' + \frac{1}{2})^2 - 204.7(\nu'' + \frac{1}{2}) + 0.3(\nu'' + \frac{1}{2})^2$. System B: $\nu_H = 15189.7 + 192.8(\nu' + \frac{1}{2}) - 0.3(\nu' + \frac{1}{2})^2 - 203.9(\nu'' + \frac{1}{2}) + 0.3(\nu'' + \frac{1}{2})^2$. System A: $\nu_H = 15047.9 + 186.2(\nu' + \frac{1}{2}) - 0.6(\nu' + \frac{1}{2})^2 - 204.7(\nu'' + \frac{1}{2}) + 0.3(\nu'' + \frac{1}{2})^2$.							NOV 1974 (1) (1) (1) (1)	
$^{197}\text{Au}^{45}\text{Sc}$		$\mu = 36.601858_6$	$D_0^0 = 2.8_7 \text{ eV}^a$						NOV 1974	
$^{197}\text{Au}^{(80)}\text{Se}$		$(\mu = 56.850286_8)$	$D_0^0 = 2.4_8 \text{ eV}^a$						NOV 1974	
(A) (15834) (X) 0		(210) ^b H (270) ^b H						(A) → (X), (15804) ^b H	(1)	
$^{197}\text{Au}^{28}\text{Si}$		$\mu = 24.4973499$	$D_0^0 = 3.2_4 \text{ eV}^a$						NOV 1974	
A ($^2\Sigma$) 13632.7 x_2 ($^2\Pi_{3/2}$) (1071) x_1 ($^2\Pi_{1/2}$) 0		389.5 ^b H 2.22 390.9 ^b H 1.32						$A \leftrightarrow x_2$, ^c (12561) H $A \leftrightarrow x_1$, R 13631.8 H	(1)(2)* (5) (1)(2)* (5)	
$^{197}\text{Au}^{(120)}\text{Sn}$		$(\mu = 74.531563_9)$ $D_0^0 = 2.4_9 \text{ eV}^a$ Fragments of an unidentified system, possibly due to AuSn, in thermal emission from 25000 to 26300 cm^{-1} .							NOV 1974	
A ($^2\Sigma$) 13899.0 x_2 ($^2\Pi_{3/2}$) (2545) x_1 ($^2\Pi_{1/2}$) 0		179.0 H 1.44 190.4 H 1.26						$A \leftrightarrow x_2$, ^b (11348) H $A \leftrightarrow x_1$, R 13893.3 H	(2) (2)(3) (2)(3)	

AuSb: (1) Houdart, Bocquet, CR B 264, 860 (1967).

AuSc: ^aThermochemical value (mass-spectrom.)(1).

- (1) Gingerich, Finkbeiner, Proc. 9th Rare Earth Res. Conf., Blacksburg Va. (October 1971). Edited by P. E. Field. Vol. II, 795.

AuSe: ^aThermochemical value (mass-spectrom.)(2).

^bPreliminary data only, no details.

- (1) Joshi, JMS 8, 79 (1962).
(2) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

AuSi: ^aThermochemical value (mass-spectrom.)(3)(4).

^b $\Delta G'(\frac{1}{2}) = 386.0$, and $\Delta G''(\frac{1}{2}) = 391.2$, from band heads acc. to (1).

^cComplex system of V and R shaded bands. No analysis.

- (1) Barrow, Gissane, Travis, Nature 201, 603 (1964).
(2) Houdart, CR B 262, 550 (1966).
(3) Gingerich, JCP 50, 5426 (1969).
(4) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart, TFS 66, 809 (1970).
(5) Houdart, Schamps, JP B 6, 2478 (1973).

AuSn: ^aThermochemical value (mass-spectrom.)(1).

^bThree sequences of bandheads. Low dispersion only.

- (1) Ackerman, Drowart, Stafford, Verhaegen, JCP 36, 1557 (1962).
(2) Collette, Schiltz, CR 257, 2092 (1963).
(3) See ref. (5) of AuSi.

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	ν ₀₀	
¹⁹⁷ Au(⁸⁸)Sr		(μ = 60.779779 ₉) Unclassified bands from 14500 to 15200 cm ⁻¹ . ^a							NOV 1974	
C	14162.2	155.6 ₃	H	0.28				C→X, ^a	14163.3 H	(1)
B	13832.7	147.04	H ^Q	0.92 ^b				B→X, ^a V	13829.4 H ^Q	(1)*
(A)		(140) ^c	H					(A→X) ^{ac}		(1)
X (2Σ)	0	153.33	H ^Q	0.19 ^d						
¹⁹⁷ Au ¹⁵⁹ Tb		μ = 87.956432 D ₀ ⁰ = 3.0 eV ^a							FEB 1975	
¹⁹⁷ Au(¹³⁰)Te		(μ = 78.278717 ₇) D ₀ ⁰ = 2.4 ₂ eV ^a							NOV 1974	
A	15481	156.1	H	0.1 ₀				A→X, R	15453 H	(1)*
(X)	0	212.5	H	0.5 ₀						
¹⁹⁷ Au ²³⁸ U		μ = 107.784312 D ₀ ⁰ = 3.2 ₅ eV ^a							NOV 1974	
¹⁹⁷ Au ⁸⁹ Y		μ = 61.256283 ₄ D ₀ ⁰ = 3.0 ₈ eV ^a							NOV 1974	

AuSr: ^aThermal emission.
^b $w_e y_e = +0.06$.
^cUncertain analysis of bands in the region 11600 -
 13200 cm^{-1} , possibly forming part of $B \rightarrow X$ (1).
^d $w_e y_e = -0.007$.
 (1) Schiltz, AP(Paris) 8, 67 (1963).

AuTb: ^aThermochemical value (mass-spectrom.)(1)(2).
 (1) Gingerich, CPL 13, 262 (1972).
 (2) Kordis, Gingerich, Seyse, JCP 61, 5114 (1974).

AuTe: ^aThermochemical value (mass-spectrom.)(2).
 (1) Maheshwari, Sharma, PPS 81, 898 (1963).
 (2) Smoes, Mandy, Vander Auwera-Mahieu, Drowart,
 BSCB 81, 45 (1972).

AuU: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, Blue, JCP 47, 5447 (1967).

AuY: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, Finkbeiner, Proc. 9th Rare Earth Res.
 Conf., Blacksburg Va. (October 1971); ed. Field.
 Vol. II, p. 795.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{11}\text{B}_2$		$\mu = 5.5046526_7$ $D_0^0 = 3.0_2 \text{ eV}^a$								SEP 1976
A $3\Sigma_u^-$	30573.4	937.4	Z 2.6	1.160	0.011		1.625	A \leftrightarrow X, R	30518.10 Z	(1)* (2)(6)
X $3\Sigma_g^-$ ^b	0	1051.3	Z 9.35	1.212	0.014		1.590			
$(^{138}\text{Ba}^{79}\text{Br})$		$(\mu = 50.194041_5)$ $D_0^0 = 3.7_9 \text{ eV}^a$								FEB 1976 A
E $2\Sigma^+$	26865.9	219.9	H 0.35					E \leftrightarrow X, V	26878.9 H	(2)(7)(8)
D $2\Sigma^+$	25670.9	209.1	H 0.53					D \leftrightarrow X, V	25678.5 H	(2)(7)(8)
C 2Π	19192.5 18650.9	197.4	H 0.41					C ^b \leftrightarrow X, R	19194.3 H 18652.7 H	(1)(2)(7)(8)
B ($2\Sigma^+$)	11325 ^c							B \rightarrow X,		(7)
A (2Π)	10604 ^c 9980 ^c							A \rightarrow X,		(7)
X $2\Sigma^+$	0	193.8	H 0.42							
$^{138}\text{Ba}^{35}\text{Cl}$		$\mu = 27.8953776$ $D_0^0 = 4.5_5 \text{ eV}^a$								FEB 1976 A
G (2Σ)	32511.4	331.3	1.29					G \leftarrow X, V	32537.3	(2)
F (2Σ)	29493.6	331.8	H 1.30					F \leftarrow X, V	29519.7 H	(2)
E $2\Sigma^+$	27064.8	311.5	H 0.93					E \leftrightarrow X, V	27080.9 H	(1)* (2)
D $2\Sigma^+$	25471.6	304.6	H 1.04					D \leftrightarrow X, V	25484.2 H	(1)* (2)
C 2Π	19450.1 19062.9	285.0 280.2	H ^Q 0.79 H ^Q 0.79					C ^b \leftrightarrow X, R _V	19453.0 H ^Q 19063.4 H ^Q	(1)* (2)
B ($2\Sigma^+$)	11880.0	255.25	H 0.83					B \leftrightarrow X, R	11868.0 H	(3)(14)
A (2Π)	10995.3 10363	256.35	H 0.73					A \leftrightarrow X, R	10983.9 H 10351.1 H	(3)(14) (8)(14)
X $2\Sigma^+$	0	279.3	H 0.89							

- B_2 : ^aThermochemical value (mass-spectrom.); from (3), but using the higher value from (5) for the heat of sublimation of boron.
- ^bExperimental evidence (6) supports a $^3\Sigma$ ground state; theoretical calculations (4) predict a $^5\Sigma_u^-$ state at approximately 1100 cm^{-1} below the lowest state of $^3\Sigma_g^-$ symmetry.
- (1) Douglas, Herzberg, CJR A 18, 165 (1940).
 - (2) Nicholls, Fraser, Jarman, CF 3, 13 (1959).
 - (3) Verhaegen, Drowart, JCP 37, 1367 (1962).
 - (4) Bender, Davidson, JCP 46, 3313 (1967).
 - (5) JANAF (1971).
 - (6) Graham, Weltner, private communication (1976); JCP 65, 1516 (1976).
- BaBr: ^aThermochemical value (flame photometry)(5). In agreement with a theoretical lower limit of 3.76 eV (3).
- ^bRadiative lifetimes (6) for the upper ($v=8$) and for the lower ($v=4$) component of $C\ ^2\Pi$ are 16.5 and 17.9 ns, respectively. A shorter lifetime of 8 ns was reported
- ^cPreliminary data, no details. | by (4).
- (1) Hedfeld, ZP 68, 610 (1931).
 - (2) Harrington, Dissertation (U. of California, 1942).
 - (3) Krasnov, Karaseva, OS(Engl. Transl.) 19, 14 (1965).
 - (4) Capelle, Bradford, Broida, CPL 21, 418 (1973).
 - (5) Gurvich, Ryabova, Khitrov, FSCS No. 8, 83 (1973); Khitrov, Ryabova, Gurvich, HT(USSR) 11, 1005 (1973).
 - (6) Dagdigian, Cruse, Zare, JCP 60, 2330 (1974).
 - (7) Bradford, Jones, Southall, Broida, JCP 62, 2060 (1975).
 - (8) Joshi, Gopal, Pramāṇa 4, 276 (1975).

- BaCl: ^aThermochemical value (mass-spectrom.)(6)(7). In agreement with a theoretical lower limit (5) of 4.35 eV. Flame photometry (11)(12) gives 4.6₃ eV. A higher value, $D_0^0 \geq 4.7_7$ eV, was estimated (9) from the short-wavelength limit of the BaCl chemiluminescence spectrum.
- ^bRadiative lifetimes (13) for the upper and the lower component of $C\ ^2\Pi(v=0)$ are 16.6 and 17.5 ns, respectively. (10) give $\tau = 22$ ns.
- (1) Parker, PR 46, 301 (1934).
 - (2) See ref. (2) of BaBr.
 - (3) Barrow, Crawford, Nature 157, 339 (1946).
 - (4) Gurvich, Ryabova, HT(USSR) 2, 190 (1964); 3, 604 (1965).
 - (5) See ref. (3) of BaBr.
 - (6) Zmbov, CPL 4, 191 (1969).
 - (7) Hildenbrand, JCP 52, 5751 (1970).
 - (8) Lagerqvist, quoted in DONNSPEC (1970).
 - (9) Jonah, Zare, CPL 2, 65 (1971).
 - (10) See ref. (4) of BaBr.
 - (11) See ref. (5) of BaBr.
 - (12) Ryabova, Khitrov, Gurvich, HT(USSR) 10, 669 (1973).
 - (13) See ref. (6) of BaBr.
 - (14) See ref. (7) of BaBr.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(138) Ba ¹⁹ F		$(\mu = 16.6980158)$		$D_0^0 = 6.05 \text{ eV}^a$		$I.P. = 4.8_5 \text{ eV}^b$				FEB 1976
I		(514)						I \rightarrow X, (33717)		(11)
H (² Σ)	31582.3	508.8	H	2.00				H \leftrightarrow X, (V) 31602.2 H		(3)(11)
G (² Σ)	31451.9	510.4	H	0.83				G \leftrightarrow X, (V) 31472.9 H		(3)(11)
F (² Σ)	29411.3	529.9	H	2.00				F \leftrightarrow X, ^c (V) 29441.8 H		(3)(11)
E ² Σ^+	28139.7	538.4	H	1.90	[0.2290] ^d	(0.0011)	[0.162]	[2.100]	E \leftrightarrow X, V 28174.45 Z	(3)(7)(11)
D' ² Σ^+	26227.0	504.9	H	1.54	0.2269 ^e	(0.00099)	0.176 ^e	2.109 ^e	D' \leftrightarrow X, V 26245.0 ^f Z	(2)* (3)(7) (9)(11)
D ² Σ^+	24156.8	508.4	H	1.88	[0.2273] ^g	(0.0011)	[0.173]	[2.107]	D \leftrightarrow X, ^h V 24176.54 Z	(2)* (3)(7) (11)
C ² Π	20197 19998.2	456.0	H	1.6 ₇	(0.2148) ⁱ (0.2138) ⁱ	(0.0012)		(2.170)	C ^j \leftrightarrow X, R 20191 H 19991.8 H	(2)* (9)(12) (13)(15)
B ² Σ^+	14062.5	424.4	H	1.88	[0.2071] ^k	(0.0012)	[0.190]	[2.208]	B \leftrightarrow X, ^c R 14040.21 Z	(1)(2)* (7) (9)
A ² Π_r	12278.2 11646.9	436.7 435.5	H ^Q H ^Q	1.82 1.68	[0.2119] [0.2118] ^l	(0.0012) (0.0011)	[0.208]	[2.183]	A \leftrightarrow X, R 12262.09 Z 11630.20 Z	(1)(2)(7)(9)
X ² Σ^+	0	468.9	H ^Q	1.79	[0.2158 ₅] ^m	(0.0012)	[0.175]	[2.162 ₇]	ESR sp. ⁿ	(10)
(138) Ba ¹ H		$(\mu = 1.00051337)$		$D_0^0 \leq 1.95 \text{ eV}^a$						FEB 1976
G ² Σ		Single band.		[3.65]				[2.15]	G \leftarrow X, V 31645	(12)
F ² Σ^+				[3.626] ^b		[114]		[2.156]	F \leftarrow X, V 30747.91 Z	(8)* (12)
C ² Σ^+	23675	1282	Z	15	3.59 ^{cde}	0.064	(100)	2.17	C \leftrightarrow X, V 23732 ^d (Z)	(6)(7)(9)*
D ² Σ^+	21885 ^f	428 ^f		4.5	1.62 ^{fgh}	0.017	(100)	3.22	D \leftrightarrow X, ⁱ R 21517 ^f	(9)
E $\begin{cases} ^2\Pi_{3/2} \\ ^2\Pi_{1/2} \end{cases}$	15055.4 14605	1228.6 [1186.7]	Z	16.9	3.560 ^j 3.486 ^j	0.075 0.072	[122] ^k [110] ^l	2.187	E \rightarrow X, V 15084.9 ^m Z 14630.1 ^m Z	(1)* (2)
B ² Σ^+	11092.4 ₄	1088.9	Z	15.4	3.266 ⁿ	0.070	111	2.308 ^o	B \rightarrow X, R 11052.51 Z	(3)(5)

BaF: ^aThermochemical value (mass-spectrom.)(4)(5)(8).

6.37 eV by flame photometry (6).

^bElectron impact appearance potential (5)(8).

^cDouble heads.

^dSpin-doubling, $|\gamma' - \gamma''| = 0.184$.

^eConstants for $v=1$. Spin-doubling, $|\gamma' - \gamma''| = 0.0091$.

^fCalc. from the origin of the 1-0 band at 26746.86 cm^{-1} .

^gSpin-doubling, $|\gamma' - \gamma''| = 0.0047$.

^hThe bands have normal structure, but the four branches have unusual intensities, the two strong branches being either R_1 and P_2 or R_2 and P_1 .

ⁱEstimates based on band head separations (12)(13).

^jRadiative lifetime $\tau(v=0) = 23.6 \text{ ns}$ (14).

^kSpin-splitting constant $\gamma = (-)0.263$.

^l Λ -type doubling, $\Delta v_{fe} = -0.258(J + \frac{1}{2})$.

^mSpin-splitting constant $\gamma = +0.00278$.

ⁿIn Ne and Ar matrices at 4 K (10).

- (1) Nevin, PPS 43, 554 (1931).
- (2) Jenkins, Harvey, PR 39, 922 (1932).
- (3) Fowler, PR 59, 645 (1941).
- (4) Blue, Green, Ehlert, Margrave, Nature 199, 804 (1963).
- (5) Ehlert, Blue, Green, Margrave, JCP 41, 2250 (1964).
- (6) Gurvich, Ryabova, HT(USSR) 2, 366 (1964).
- (7) Barrow, Bastin, Longborough, PPS 92, 518 (1967).
- (8) Hildenbrand, JCP 48, 3657 (1968).
- (9) Mohanty, Mohanty, Mohanty, IJPAP 8, 423 (1970).
- (10) Knight, Easley, Weltner, Wilson, JCP 54, 322 (1971).
- (11) Singh, Mohan, JP B 4, 1395 (1971); IJPAP 11, 918 (1973).
- (12) Kushawaha, Asthana, Shanker, Pathak, SpL 5, 407 (1972); Kushawaha, SpL 6, 633 (1973).
- (13) Cruse, Dagdigidian, Zare, FDCS No. 55, 277 (1973).
- (14) See ref. (6) of BaBr.
- (15) See ref. (7) of BaBr.

Ba¹H: ^aFrom the predissociation in $C \ ^2\Sigma^+(v=1)$, assuming dissociation into $^3D_3 + ^2S$; see (9).

^bDiffuse lines.

^cSpin-splitting constant $\gamma = +0.14$.

^d $v=0$ interacts strongly with successive vibrational levels of $D \ ^2\Sigma^+$. A third (unidentified) state affects the low J levels in $v=0$; see (9).

^eEmission from $v=1$ breaks off above $N=8$; in absorption, the lines become broad for $N' \geq 10$. Similar predissociation effects in absorption to $v'=2$ and 3; see (9).

^fVibrational numbering uncertain.

^gSpin-splitting constant $\gamma = +0.12$.

^hStrong interactions with $C \ ^2\Sigma^+(v=0)$. Weaker perturbations may be caused by a $^4\Sigma$ state; for details see Figs. 6 and 10 of (9).

ⁱThe P_2 and R_1 branches are about twice as strong as the P_1 and R_2 branches (9)(11).

^jSmall perturbations. Large Λ -type doubling in $^2\Pi_{\frac{1}{2}}$. For a refined treatment of the rotational structure see (15).

^k $H_0 = +3.1 \times 10^{-9}$.

^l $H_0 = +2.0 \times 10^{-9}$.

^m $\{J'=0\}$ relative to $N''=0$.

ⁿEffective constants. Very large spin doubling ($\gamma_0 \approx -4.9$) due to interaction with $A \ ^2\Pi$. "True" constants ($B_e = 3.164$, $\alpha_e = 0.061$) have been determined by (16) whose revised spin splitting parameters are in good agreement with "pure precession" values for $l=2$.

^oFrom the "true" rotational constants; see ⁿ and ^p.

(continued p.68)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(139) Ba ¹ H (continued)										
A $\begin{cases} 2\Pi_{3/2} \\ 2\Pi_{1/2} \end{cases}$	$\begin{matrix} 9939.82 \\ 9457.45 \end{matrix}$	$\begin{matrix} 1109.9_8 \\ 1110.55 \end{matrix}$	$\begin{matrix} Z & 13.59 \\ Z & 15.29 \end{matrix}$	$\begin{matrix} 3.322^{\text{pq}} \\ 3.27887^{\text{p}} \end{matrix}$	$\begin{matrix} 0.082 \\ 0.07283 \end{matrix}$	$\begin{matrix} [132.2]^{\text{r}} \\ [121]^{\text{s}} \end{matrix}$	2.249^{o}	A \leftrightarrow X, R	$\begin{matrix} 9910.88^{\text{m}} Z \\ 9428.37^{\text{m}} Z \end{matrix}$	$\begin{matrix} (4)(5)(10) \\ (10)(16) \end{matrix}$
H ($2\Delta_{3/2}$)	$[10609]^{\text{t}}$	$[1023]^{\text{t}}$		$[2.97]^{\text{t}}$						(14)
X $2\Sigma^+$	0	1168.31	Z 14.50	3.38285^{u}	0.06599	$[112.67]^{\text{v}}$	2.23175	ESR sp. ^w		(14)
(138) Ba ² H										
		$(\mu = 1.98510975)$		$D_0^0 \leq 1.97 \text{ eV}^{\text{a}}$						FEB 1976
F $2\Sigma^+$	(30708)	$[860.6]$	Z	$[1.8376]^{\text{b}}$	^c	$[29.2]$	$[2.1497]$	F \leftarrow X, V	30725.25 Z	(1)(6)(7)
C $2\Sigma^+$	23675	910	7.6	1.80^{d}	0.020		2.17	C \leftarrow X, V	23715	(2)* (7)
D $2\Sigma^+$	21884 ^e	304 ^e	(2.3)	0.827^{ef}	(0.008 ₂)		3.20	D \leftarrow X, R	21622 ^e	(2)(7)
E $\begin{cases} 2\Pi_{3/2} \\ 2\Pi_{1/2} \end{cases}$	$\begin{matrix} 15059.32 \\ 14604.12 \end{matrix}$	$\begin{matrix} 872.19 \\ 867.82 \end{matrix}$	$\begin{matrix} Z & 8.47 \\ Z & 8.78 \end{matrix}$	$\begin{matrix} 1.7874^{\text{gh}} \\ 1.7653^{\text{gi}} \end{matrix}$	$\begin{matrix} 0.0259 \\ 0.0255 \end{matrix}$	$\begin{matrix} [30.4]^{\text{j}} \\ [28.4] \end{matrix}$	2.186	E \leftarrow X, V	$\begin{matrix} 15080.24^{\text{k}} Z \\ 14622.78^{\text{k}} Z \end{matrix}$	$\begin{matrix} (7)* \\ (7)* \end{matrix}$
B $2\Sigma^+$	11089.62	772.99	Z 7.72	1.6355^{l}	0.0252	$[28.9]^{\text{m}}$	2.298^{n}	B \leftarrow X, R	11061.13 Z	(3)* (7)
A $\begin{cases} 2\Pi_{3/2} \\ 2\Pi_{1/2} \end{cases}$	$\begin{matrix} 9938.34 \\ 9456.20 \end{matrix}$	$\begin{matrix} 791.23 \\ 788.85 \end{matrix}$	$\begin{matrix} Z & 7.80 \\ Z & 7.67 \end{matrix}$	$\begin{matrix} 1.65983^{\text{o}} \\ 1.6475^{\text{oq}} \end{matrix}$	$\begin{matrix} 0.02710 \\ 0.0259 \end{matrix}$	$\begin{matrix} [31.0]^{\text{p}} \\ [29.4] \end{matrix}$	2.259^{n}	A \leftarrow X, R	$\begin{matrix} 9918.95^{\text{k}} Z \\ 9435.65^{\text{k}} Z \end{matrix}$	$\begin{matrix} (4)* (7) \\ (4)(7)(10) \end{matrix}$
H ($2\Delta_{3/2}$)	$[9840]^{\text{r}}$			$[1.591]^{\text{r}}$						
X $2\Sigma^+$	0	829.77	Z 7.32	1.7071^{s}	0.02363	$[28.77]^{\text{t}}$	2.2304			

Ba¹H (continued):

^pEffective constants. Large Λ -type doubling due to interaction with B $2\Sigma^+$;

$$2\Pi_{3/2}, \Delta v_{fe}(v=0) = -3.38 \times 10^{-4} (J - \frac{1}{2})(J + \frac{1}{2})(J + \frac{3}{2}) + \dots;$$

$$2\Pi_{1/2}, \Delta v_{fe}(v=0) = -5.307 (J + \frac{1}{2}) + \dots$$

(16) has evaluated "true" constants for $v=0,1,2$ ($A_0 = +438.1$, $B_0 = 3.306$, ...) and has shown that the Λ -type

Ba¹H (continued):

doubling agrees with "pure precession" values for $l=2$.

^qPerturbations by H $2\Delta_{3/2}(v \geq 2)$ (10)(16).

$$r_{H_0} = +6.6 \times 10^{-9}.$$

$$s_{H_0} = +4 \times 10^{-9}.$$

^tConstants (10) for the lowest observed level, probably $v=2$ (16). From perturbations in A $2\Pi_{3/2}$.

Ba¹H (continued):

^uSpin splitting constant $\gamma_0 = +0.1927$; also higher order terms (10)(13).

^v $H_0 = +2.89 \times 10^{-9}$.

^wIn Ar matrix at 4 K (14).

(1) Fredrickson, Watson, PR 39, 753 (1932).

(2) Funke, ZP 84, 610 (1933).

(3) Watson, PR 43, 9 (1933).

(4) Watson, PR 47, 213 (1935).

(5) Koontz, Watson, PR 48, 937 (1935).

(6) Grundström, ZP 92, 595 (1936).

(7) Funke, Grundström, ZP 100, 293 (1936).

(8) Edvinsson, Kopp, Lindgren, Åslund, AF 25, 95 (1963).

(9) Kopp, Åslund, Edvinsson, Lindgren, AF 30, 321 (1965).

(10) Kopp, Kronekvist, Guntzsch, AF 32, 371 (1966).

(11) Kopp, Hougen, CJP 45, 2581 (1967).

(12) Khan, JP B 1, 985 (1968).

(13) Veseth, JP B 3, 1677 (1970).

(14) Knight, Weltner, JCP 54, 3875 (1971).

(15) Veseth, JMS 38, 228 (1971).

(16) Veseth, MP 20, 1057; 21, 287 (1971); 25, 333 (1973).

Ba²H: ^aSee ^a of Ba¹H.

^bSee ^b of Ba¹H.

^c $v=1$ perturbed, $B_1 \approx 1.855$, $D_1 \approx 41 \times 10^{-6}$.

^dStrong interactions with $D^2\Sigma^+$. Only $v=1$ has been analyzed in detail. Lines are broad above $v'=1, N'=22$.

^eSee ^f of Ba¹H.

^fStrong interactions with $C^2\Sigma^+$. $v=8...11$ have been analyzed, but only $v=11$ has been deperturbed.

^gEffective constants. For a refined treatment of the ro-

Ba²H (continued):

tational structure see (9).

^h Λ -type doubling,

$\Delta v_{fe}(v=0) = +0.060 \times 10^{-4} (J-\frac{1}{2})(J+\frac{1}{2})(J+\frac{3}{2}) - \dots$

ⁱ Λ -type doubling, $\Delta v_{fe}(v=0) = +0.433(J+\frac{1}{2}) - \dots$. $v=0$ is perturbed by $B^2\Sigma^+(v=5)$.

^j $H_0 = +4.1 \times 10^{-10}$.

^kSee ^m of Ba¹H.

^lEffective constants. Very large spin splitting, $\gamma_0 = -2.433$. "True" constants ($B_e = 1.608$, $\alpha_e = 0.024$) have been evaluated (10); see ⁿ of Ba¹H.

^m $H_0 = +3.7 \times 10^{-10}$.

ⁿFrom the "true" rotational constants; see ^l and ^o.

^oEffective constants. Large Λ -type doubling:

$2\Pi_{3/2}$, $\Delta v_{fe}(v=0) = -0.524 \times 10^{-4} (J-\frac{1}{2})(J+\frac{1}{2})(J+\frac{3}{2}) + \dots$;

$2\Pi_{1/2}$, $\Delta v_{fe}(v=0) = -2.636(J+\frac{1}{2}) + \dots$; see also (5).

"True" constants for $v=0,1,2$ ($A_0 = +433.6$, $B_0 = 1.652$, ...) have been evaluated (10); see ^p of Ba¹H.

^p $H_0 = +5.3 \times 10^{-10}$.

^q $v=0$ perturbed by $H^2\Delta_{3/2}(v=2)$.

^rSingle level, probably $v=2$ (10), observed in a perturbation of $A^2\Pi_{1/2}(v=0)$.

^sSpin splitting constant $\gamma_0 = +0.0972$; also higher order terms (7)(8).

^t $H_0 = +4.0 \times 10^{-10}$.

(1) See ref. (8) of Ba¹H.

(2) See ref. (9) of Ba¹H.

(3) Kopp, Wirhed, AF 32, 307 (1966).

(4) See ref. (10) of Ba¹H.

(continued p. 71)

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	ν ₀₀	
(138) Ba ¹²⁷ I		(μ = 66.088178 _g) D ₀ ⁰ = 4.42 eV ^a Additional emission bands in the region 22300 - 23300 cm ⁻¹ , ν _e = $\frac{23224.8}{22664.7}$ ω _e ' = $\frac{173.0}{171.0}$ ω _e 'x _e ' = $\frac{0.50}{0.50}$ ω _e '' = $\frac{177.0}{177.0}$ ω _e ''x _e '' = $\frac{0.60}{0.65}$								SEP 1976
E (2Σ ⁺)	26753	176.0 ^b	H 0.30					E↔ X, V	26765	H (4)(5)(6)*
D (2Σ ⁺)	25764	161.1 ^b	H 0.26					D↔ X, V	25769 ^b	H (4)(5)(6)*
C (2Π)	18569 17814	150.05 ^c	H 0.275					C ^d ↔ X, ν _R	18568 17813	H (1)(2)(4)(5) H (12)
B (2Σ)	10417 ^e							B→ X,		(10)
A (2Π)	9921 ^e 9268 ^e							A→ X,		(10)
X (2Σ ⁺)	0	152.30 ^c	H 0.270							

Ba²H (continued):

- (5) See ref. (11) of Ba¹H.
- (6) See ref. (12) of Ba¹H.
- (7) Kopp, Wirhed, AF 38, 277 (1968).
- (8) See ref. (13) of Ba¹H.
- (9) See ref. (15) of Ba¹H.
- (10) See ref. (16) of Ba¹H.

- BaI: ^aFrom the Ba + I₂ chemiluminescence spectrum, see (11).
Lower bounds were earlier predicted by (3) and (7).
^bVibrational constants from (4). Similar results in (5).
A different analysis of the D-X system has been suggested (6), placing the 0-0 band at 26101 cm⁻¹, and resulting in increased upper and lower state vibrational constants.
^cVibrational constants recalculated by (12) from unpublished data of M. M. Patel; for the upper state there is only moderate agreement with the constants in (4).
^dRadiative lifetime $\tau = 16.5$ ns (9).
^ePreliminary data, no details.
- (1) Walters, Barratt, PRS A 118, 120 (1928).
 - (2) Mesnage, AP(Paris) 12, 5 (1939).
 - (3) See ref. (3) of BaBr.
 - (4) E. Morgan, unpublished, quoted in DONNSPEC (1970).
 - (5) Patel, Shah, IJPAP 8, 681 (1970).
 - (6) Reddy, Rao, JP B 3, 1008 (1970).
 - (7) Mims, Lin, Herm, JCP 57, 3099 (1972).
 - (8) Shah, Patel, Darji, JP B 5, L191 (1972).
 - (9) See ref. (6) of BaBr.
 - (10) See ref. (7) of BaBr.
 - (11) Dickson, Kinney, Zare, CP 15, 243 (1976).
 - (12) Dagdigian, Cruse, Zare, CP 15, 249 (1976).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{138}\text{Ba}^{160}$ [36490 - 38620]		$\mu = 14.3325559_8$ $D_0^0 = 5.79 \text{ eV}^a$ I.P. = 6.9_1 eV^b Nineteen $^1\Sigma^+$ vibronic levels belonging to two or more perturbed electronic states. ^c								SEP 1976 A (35)
B ($^1\Pi$)	32866.4	488	H	3.6					B \leftrightarrow X, R 32775	H (5)*
A' $^1\Pi$ d	17691	443	H	1.66	0.2252 ^e	0.0013 ₀	(2.3)	2.285	A', ^f \leftrightarrow X, R 17578	H (32)(34) (39)* (40)
a $\left\{ \begin{array}{l} 3\Pi_0^+ \\ 3\Pi_1 \\ 3\Pi_2 \end{array} \right.$ d	17586.5	449.0 ^g		2.5	0.2254 ₄ ^g	0.0013 ₈				
	17442	[445] ^g		(4.5)	[0.2254] ₄ ^g			2.289		
	17393	^g			^g					
A $^1\Sigma^+$	16807.2	499.7 ^h	Z	1.6 ₄	0.25832 ^h	0.001070	2.8	2.1338	A ⁱ \leftrightarrow X, ^j R 16722.25 Z	(1)* (2)* (4)* (18) (31)
									Microwave optical double resonance	(22)(23)(26)
X $^1\Sigma^+$	0	669.76 ^k	Z	2.02 ₈ ^l	0.3126140 ^k	0.0013921 ^m	2.724	1.939692 ⁿ	Microwave sp. ^o Mol. beam electric ^p and magn. reson. ^q	(7)(15)(33) (6) (10)

BaO: ^aBy extrapolation of the highest observed ground state levels ($v=0, J$) populated in the reaction $\text{Ba} + \text{CO}_2$ under single-collision conditions (31). Compatible with lower bounds obtained from the short-wavelength limits of the $\text{Ba} + \text{NO}_2$ (17)(21) and $\text{Ba} + \text{ClO}_2$ (40) chemiluminescence spectra. Flame photometric values (16)(27)(36), if corrected to a $^1\Sigma$ ground state, are near 5.6₉ eV. Earlier measurements reviewed in (12)(13).

^bElectron impact appearance potential (28)(38).

^cOptical-optical double resonance laser spectroscopy.

^d $^3\Pi_2$, $^3\Pi_1$, $^3\Pi_0$, and $^1\Pi$ [see (29)] correspond to Q, Z, Y, and X, respectively, of (2)(3).

^eOnly $v=12, 17, 18$ have been rotationally analyzed (34). In addition, constants for $v=2, 3, 4$ have been derived (2)(3) from perturbations (29) in $v=3, 4, 5$, resp., of A $^1\Sigma^+$.

^fRadiative lifetime $\tau(v=13\dots 17) = 9 \mu\text{s}$ (34). Similar lifetimes observed by (18)(20) can be attributed to either A' $^1\Pi$ or a $^3\Pi_1$; see (30).

^gFrom perturbations in A $^1\Sigma^+$ (2)(3)(29). (29) has adopted the following constants for a $^3\Pi_1$: $T_e = 17483$, $A = -105$, $\omega_e = 448.3$, $\omega_e x_e = 2.39$, $B_e = 0.2244$, $\alpha_e = 0.0014$.

^hPartially deperturbed constants. Numerous interactions with levels of a $^3\Pi_1$ and A' $^1\Pi$, except in $v=0$ which is unperturbed (2)(3)(29). Potential curve (11)(37).

BaO (continued):

ⁱRadiative lifetime $\tau(v=0) = 0.356 \mu s$; $f_{00}(A \leftarrow X) = 0.00026$ (20). Slight variation of τ with v .

^jRelative intensities (9)(14)(19)(25); Franck-Condon factors (8)(24)(37).

^kThe ground state constants have been derived (35) from a combination of microwave rotational constants (15)(33), electronic band origins (2), and data on higher vibrational levels ($v \leq 34$) obtained by optical-optical double resonance photoluminescence spectroscopy. They were used for the construction of the RKR potential curve up to $v=40$ (35).

^l $w_{e y_e} = -0.0035$, $w_{e z_e} = -6.3 \times 10^{-5}$.

^m $r_e = -4.33 \times 10^{-6}$.

ⁿFrom the Dunham corrected microwave B_e value in (33).

^oValues of $eqQ(^{135,137}\text{Ba})$ in (15)(33).

^p $\mu_{e l}(v) = [7.934 + 0.042(v + \frac{1}{2})] D$.

^q $g_J = (-)0.103$.

- (1) Mahanti, PPS 46, 51 (1934).
- (2) Barrow, Lagerqvist, Lind, Nature 164, 923 (1949); Lagerqvist, Lind, Barrow, PPS A 63, 1132 (1950).
- (3) Kovács, Lagerqvist, JCP 18, 1683 (1950); AF 2, 411 (1950).
- (4) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (5) Parkinson, PPS 78, 705 (1961).
- (6) Wharton, Kaufman, Klemperer, JCP 37, 621 (1962); 39, 240 (1963).
- (7) Wharton, Klemperer, JCP 38, 2705 (1963).
- (8) Ortenberg, Glasko, Dimitriev, SAAJ 8, 258 (1964).
- (9) Vaidya, Desai, Bidaye, JQSRT 4, 353 (1964).
- (10) Brooks, Kaufman, JCP 43, 3406 (1965).
- (11) Singh, Rai, IJPAP 4, 102 (1966).
- (12) Schofield, CRev 67, 707 (1967).

- (13) Gaydon, DISSEN (1968), p. 241.
- (14) Walvekar, Korwar, JP B 2, 115 (1969).
- (15) Hoefl, Lovas, Tiemann, Törring, ZN 25 a, 1750 (1970).
- (16) Kalff, Alkemade, JCP 52, 1006 (1970).
- (17) Ottinger, Zare, CPL 5, 243 (1970).
- (18) Sakurai, Johnson, Broida, JCP 52, 1625 (1970).
- (19) Degen, Brown, Romick, PSS 19, 1625 (1971).
- (20) Johnson, JCP 56, 149 (1972).
- (21) Jonah, Zare, Ottinger, JCP 56, 263 (1972).
- (22) Field, Bradford, Harris, Broida, JCP 56, 4712 (1972).
- (23) Field, Bradford, Broida, Harris, JCP 57, 2209 (1972).
- (24) Wentink, Spindler, JQSRT 12, 129 (1972).
- (25) Best, Hoffman, JQSRT 13, 69 (1973).
- (26) Field, English, Tanaka, Harris, Jennings, JCP 59, 2191 (1973).
- (27) Kalff, Alkemade, JCP 59, 2572 (1973); 60, 1698 (1974).
- (28) Panchenkov, Gusarov, Gorokhov, RJPC 47, 55 (1973).
- (29) Field, JCP 60, 2400 (1974).
- (30) Field, Jones, Broida, JCP 60, 4377 (1974).
- (31) Dagdigian, Cruse, Schultz, Zare, JCP 61, 4450 (1974).
- (32) Hsu, Krugh, Palmer, Obenauf, Aten, JMS 53, 273 (1974).
- (33) Tiemann, Bojaschewsky, Sauter-Servaes, Törring, ZN 29 a, 1692 (1974).
- (34) Pruett, Zare, JCP 62, 2050 (1975).
- (35) Field, Capelle, Revelli, JCP 63, 3228 (1975).
- (36) Van der Hurk, Hollander, Alkemade, JQSRT 15, 113 (1975).
- (37) Tawde, Tulasigeri, APH 38, 299 (1975).
- (38) Rauh, Ackermann, JCP 64, 1862 (1976).
- (39) Wyss, Broida, JMS 59, 235 (1976).
- (40) Engelke, Sander, Zare, JCP 65, 1146 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{138}\text{Ba}^{32}\text{S}$										
		$\mu = 25.9547097$ $D_0^0 = 4.36 \text{ eV}^a$								MAR 1976 A
B $1\Sigma^+$	27060.29	254.10	Z 0.438	0.08604	0.00044		2.747 ₅	B \leftarrow X, R	26997.74 Z	(5)
A $1\Sigma^+$	14493	294. ₃ ^b	3.0 ₈	0.0935 ₃ ^b	0.0007 ₂		2.635	A \leftarrow X, R	14450	(3)(5)
a ($3\Pi_0^+$)	(14570)	(235) ^c		(0.078 ₅) ^c			(2.88)			
X $1\Sigma^+$	0	379.42	Z 0.8842	0.10331	0.0003188	0.306	2.5074	Mol. beam el. reson. ^d		(4)
$^{11}\text{B}^{79}\text{Br}$										
		$\mu = 9.6615016_1$ $D_0^0 = 4.49 \text{ eV}^a$								MAR 1976
A 1Π	33935.3	637.63	H ^Q 17.58 ^{bc}	[0.496] ^d	(0.0090)	[12.8]	1.87	A ^e \leftrightarrow X, v_R	33908.6 H ^Q	(1)* (2)* (6)
a $\begin{cases} 3\Pi_2 \\ 3\Pi_1 \\ 3\Pi_0^+ \end{cases}$	$\begin{cases} 18851.4_8 \\ 18673.8_3 \end{cases}$	$\begin{cases} 757.10 \\ 759.8_0 \end{cases}$	$\begin{cases} \text{H}^Q \\ 4.8_0 \end{cases}$	$\begin{cases} 4.81^f \\ 4.8_0 \end{cases}$	$\begin{cases} 0.5083^d \\ 0.5062^d \end{cases}$	$\begin{cases} 0.0036 \\ 0.0036 \end{cases}$	$\begin{cases} [9.3] \\ 1.853 \end{cases}$	a \rightarrow X, V	$\begin{cases} 18887.5_5 \text{ Z} \\ 18711.2_5 \text{ Z} \end{cases}$	(5)* (7)*
X $1\Sigma^+$	0	684.31	H ^Q 3.52	0.4894 ^d	0.0035	10.0	1.888 ₂			
$^{(11)}\text{B}^{12}\text{C}$										
		$(\mu = 5.74166243)$ $D_0^0 = 4.6_0 \text{ eV}^a$ Theoretical calculations (2) predict a $4\Sigma^-$ ground state.								MAR 1976
$^{11}\text{B}^{35}\text{Cl}$										
		$\mu = 8.3731666_4$ $D_0^0 = 5.5 \text{ eV}^a$								MAR 1976
A 1Π	36750.92	849.04	H ^Q 11.37 ^b	0.7054 ^c	0.00820 ^d	16.0 ^e	1.689 ₄	A ^f \leftrightarrow X, v_R	36754.30 H ^Q	(1)(2)(3)* (5)(6)* (7) (10)
a $3\Pi_1$	20200	911	5.7	0.698 ₆	0.004 ₇		1.698	a \rightarrow X, V	20235.7 ₀ Z	(11)
X $1\Sigma^+$	0	839.12	H ^Q 5.11	0.6838 ^c	0.00646	17.2 ^g	1.715 ₉			

BaS: ^aThermochemical value (mass-spectrom.)(2), corrected to a $^1\Sigma$ ground state.

^bExtensive perturbations arising from successive vibrational levels of three perturbing states or sub-states of smaller B values.

^cFrom perturbations in A $^1\Sigma^+$; vibrational numbering unknown.

^d $\mu_{el}(v) = [10.853 + 0.021(v + \frac{1}{2})] D$.

(1) Barrow, Gissane, Rose, PPS 84, 1035 (1964).

(2) Colin, Goldfinger, Jeunehomme, TFS 60, 306 (1964).

(3) Clements, Barrow, CC (1968), 1408.

(4) Melendres, Hebert, Street, JCP 51, 855 (1969).

(5) Barrow, Burton, Jones, TFS 67, 902 (1971).

BBr: ^aFrom the predissociation in A $^1\Pi$; see (3).

^b $w_{ey_e} = + 1.10$, $w_{ez_e} = - 0.250$. This state may have a potential hump of ~ 0.13 eV; see (3).

^cPredissociation above $v = 4$ (1).

^dThe rotational constants refer to the normal $^{79,81}\text{Br}$ isotopic mixture.

^eRadiative lifetime $\tau(v=0, 1) = 26$ ns (4), corresponding to an absorption f_{00} value of 0.10.

^f $w_{ey_e} \approx - 0.004$.

(1) Miescher, HPA 8, 279 (1935); 9, 693 (1936).

(2) Rosenthaler, HPA 13, 355 (1940).

(3) Barrow, TFS 56, 952 (1960).

(4) Lutz, Hesser, JCP 48, 3042 (1968).

(5) Lebreton, Marsigny, Bosser, CR C 271, 1113 (1970).

(6) Wentink, Spindler, JQSRT 10, 609 (1970).

(7) Lebreton, JCPPB 70, 738 (1973).

BC: ^aThermochemical value (mass-spectrom.)(1).

(1) Verhaegen, Stafford, Drowart, JCP 40, 1622 (1964).

(2) Kouba, Öhrn, JCP 53, 3923 (1970).

BCI: ^aExtrapolation of A $^1\Pi$; see (4).

^b $w_{ey_e} = - 0.100$, $w_{ez_e} = - 0.0271$.

^cRKR potential curve (8).

^d $f_e = - 0.00050$.

^e $\beta_e = + 2.7 \times 10^{-7}$.

^fRadiative lifetime $\tau(v=0, 1, 2) = 19.1$ ns (9); $f_{00}(A \leftarrow X) = 0.11$.

^g $\beta_e = + 0.7 \times 10^{-7}$.

(1) Jevons, PRS A 106, 174 (1924).

(2) See ref. (1) of BBr.

(3) Herzberg, Hushley, CJR A 19, 127 (1941).

(4) See ref. (3) of BBr.

(5) Thrush, Nature 186, 1044 (1960).

(6) Verma, JMS 7, 145 (1961); CJP 40, 1852 (1962).

(7) Pannetier, Goudmand, Dessaux, Arditi, CR 258, 1201 (1964).

(8) Gélébart, Johannin-Gilles, CR B 267, 408 (1968).

(9) Hesser, JCP 48, 2518 (1968).

(10) See ref. (6) of BBr.

(11) Lebreton, Marsigny, Ferran, CR C 272, 1094 (1971).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
${}^9\text{Be}_2$		$\mu = 4.5060914$								APR 1976
A ($1\Sigma_u^+$)		502 ^a	6.8					A \leftarrow X,	28551 ^a	(2)
X $1\Sigma_g^+$		483 ^b	4.5						27670 ^b	
Theoretical calculations give no evidence for a bound ground state (1).										
${}^9\text{Be}^{40}\text{Ar}^+$		$\mu = 7.3534172^a$								APR 1976 A
A $2\Pi_r$	(24605) (24563)	[570]	H			0.6127 ^b		1.934	A \rightarrow X, V 24708 24666	H H (1)(2)*
X $2\Sigma^+$	0	369	H 11			0.5271 ^b		2.085		
${}^9\text{Be}^{(79)}\text{Br}$		$(\mu = 8.0885053)$								APR 1976
A $2\Pi_r$	26554 26353 ^a	695 702	H H	5.2 4.4		[0.5332] ^b	[1.31]	[1.976]	A \rightarrow X, R 26543.3 26346.1	H H (1)(2)* (3)*
X $2\Sigma^+$	0	715	H	3.8		[0.5459] ^c	[1.31]	[1.953]		
${}^9\text{Be}^{35}\text{Cl}$		$\mu = 7.1654906$ D_0^0 ^a								SEP 1976
R shaded emission bands in the region 37900 - 38300 cm^{-1} (3) are due to AlCl . Unidentified system ($v_e = 18686$, $w_e' = 540$, $w_e'' = 552$) in emission (1); assignment to BeCl not confirmed.										
B $2\Sigma^+$	(48773)	[952.5]	Z	b		0.7751	0.0043	[3.0] ^c	1.7422	B \rightarrow X, V 48827.6 Z (6)* (8)*
A $2\Pi_r$	27992.0 ^d	822.11	Z	5.24		0.7094 ^e	0.0068	2.3	1.8211	A \leftrightarrow X, R 27979.63 (2)* (3)(5)*
X $2\Sigma^+$	0	846.7	Z	4.8 ₅		0.7285	0.0069	2.5	1.7971	
${}^9\text{Be}^{19}\text{F}$		$\mu = 6.1125850$ $D_0^0 = 5.85$ or 6.26 eV^a								APR 1976 A
R shaded double-headed emission bands in the regions 62900 - 64100 and 65800 - 66700 cm^{-1} .										
C $2\Sigma^+$	50364.0	1419.7	H	9.9		1.570	0.01 ₄		1.325	C \rightarrow A, V 17253.7 (6)
B $2\Sigma^+$	49563.9	1350.8	H	12.6		[1.54 ₇]			[1.33 ₅]	C \rightarrow X, V 50440.86 Z (9)*
A $2\Pi_r$	33233.7 ^b	[1154.67]	Z	8.78 ^c H ^q		1.4202 ₄ ^d	0.0175	[8.40] ^e	1.3935	B \rightarrow X, V 49605.6 Z (9)*
X $2\Sigma^+$	0	[1247.36]	Z	9.12 ^c H ^q		1.4889 ₃	0.0176	8.28	1.3610	A \leftrightarrow X, R 33187.13 ^f Z (1)*(2)* (3) (4)(5)(13)

Be₂: ^aIn Ne matrix at 4 K.

^bIn Ar matrix at 4 K.

(1) Bender, Davidson, JCP 47, 4972 (1967).

(2) Brom, Hewett, Weltner, JCP 62, 3122 (1975).

BeAr⁺: ^aReduced mass of Be⁺ + Ar.

^bPreliminary results.

(1) Subbaram, Vasudev, Jones, JOSA 65, 318 (1975).

(2) Subbaram, Coxon, Jones, CJP 53, 2016 (1975).

BeBr: ^aA₀ = +198.0.

^bΛ-type doubling in ²Π_{1/2}, Δv_{ef}(v=0) = (+)0.030(J+¹/₂); details in (3).

^cSpin splitting constant γ₀ = +0.0242.

(1) Reddy, Rao, JP B 1, 482 (1968).

(2) Reddy, Reddy, Rao, JP B 3, L1 (1970).

(3) Carleer, Herman, Colin, CJP 53, 1321 (1975).

BeCl: ^aThermochemical values for D₀⁰ obtained by various methods have been summarized in (7), all being close to 4.51 eV and substantially higher than a mass-spectrometric value of 3.99 eV (4). The interpretation (8) of an inverse predissociation assumed to be responsible for the strikingly high intensity of B→X bands with v'=1 suggests an even lower value of 3.45 eV.

^bA very weak head at 48502.7 cm⁻¹ has tentatively been identified as 2-3 band; ΔG'(3/2) = 1212.7 cm⁻¹.

^cD₁ = 1.9 × 10⁻⁶.

^dA_v = +52.8 - 1.4(v+¹/₂).

^eThe Λ-type doubling in the ¹/₂ [Δv_{ef}(v=0) ≈ -0.011(J+¹/₂)] and ³/₂ components does not conform with the "pure precession" pattern frequently observed in regular ²Π states; see (5).

BeCl (continued):

(1) Parker, PR 45, 752 (1934).

(2) Fredrickson, Hogan, PR 46, 454 (1934).

(3) Novikov, Tunitskii, OS(Engl. Transl.) 8, 396 (1960).

(4) Hildenbrand, Theard, JCP 50, 5350 (1969).

(5) Colin, Carleer, Prévot, CJP 50, 171 (1972).

(6) Burtin, Thèse (U. Libre de Bruxelles, 1974).

(7) Farber, Srivastava, JCS FT I 70, 1581 (1974).

(8) Carleer, Burtin, Colin, CJP 55, 582 (1977).

BeF: ^aMass-spectrometric values (7)(16).

^bA₀ = +21.82, A₁ = +21.93; slight J dependence. A negative value of A has been ruled out by the calculations of (14).

^cSlightly different constants in (5).

^dThe Λ-type doubling in the ¹/₂ and ³/₂ components (13) does not follow the "pure precession" pattern for a regular ²Π state. An earlier explanation (10) of this "anomaly" has since been revised (14).

^eD₁ = 8.26 × 10⁻⁶.

^fJ'=¹/₂ (average of F₁ and {F₂}) relative to N'=0.

(1) Jevons, PRS A 122, 211 (1929).

(2) Jenkins, PR 35, 315 (1930).

(3) Mulliken, PR 38, 836 (1931).

(4) Fowler, PR 59, 645 (1941).

(5) Tatevskii, Tunitskii, Novikov, OS 5, 520 (1958).

(6) Rao, Rao, IJPAP 3, 177 (1965).

(7) Hildenbrand, Murad, JCP 44, 1524 (1966).

(8) Singh, Rai, IJPAP 4, 102 (1966).

(9) Novikov, Gurvich, OS(Engl. Transl.) 23, 173 (1967).

(10) Walker, Richards, PPS 92, 285 (1967).

(11) Katti, Sharma, IJPAP 6, 458 (1968).

(continued p. 79)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^9\text{Be}^1\text{H}$										
		$\mu = 0.90645687$	$D_0^0 = 2.034 \text{ eV}^a$		$\text{I.P.} = 8.21 \text{ eV}^b$				SEP 1976	
G $^2\Pi$	58711	405.3	Z 22.7	5.02 ^{cd}	-0.556 ^e	[18] ^f	1.92 ₅	G \leftarrow X, R	57886.2 Z	(13)*
F $^2\Sigma^+(4p\sigma)$	(56606)	(2153) ^g		[10.576] ^h		[8.0] ^f	[1.326]	F \leftarrow X,	56661.24 Z	(13)*
E $^2\Sigma^+(4s\sigma)$	(54134)	(1970) ^g		[10.578] ⁱ		[22.4] ^f	[1.326]	E \leftarrow X,	54097.6 Z	(13)*
D $\begin{cases} ^2\Sigma^+ \\ ^2\Delta \end{cases}$	(3d) (54000)	Strong absorption, complex structure.						D \leftarrow X,	54050	(13)*
B $^2\Pi$ (3p π)	50882 ^j	2265.94	Z 71.52	10.8495 ^{kld}	0.1016 ^m	[10.35] ^f	1.3092	B \leftrightarrow X, v_R	50976.17 Z	(3)(13)*
A $^2\Pi_r$ (2p π)	20033.19 ⁿ	2088.58 ^o	Z 40.14 ^p	10.4567 ^q	0.3222 ^r	10.41 ^s	1.3336	A \leftrightarrow X, $t v^u$	20045.81 ^o Z	(1)* (2)(9)*
X $^2\Sigma^+(2p\sigma)$	0	2060.78 ^o	Z 36.31 ^v	10.3164 ^w	0.3030 ^x	10.221 ^y	1.3426	ESR sp. ^z		(10)
For theoretical calculations see references in (9)(11)(14).										

Be^1H : ^aFrom the predissociation by rotation (13) in the B' $^2\Pi$, $v'+1$ level (see ^l), assuming dissociation into $\text{Be}(^1\text{P}) + \text{H}(^2\text{S})$. The experimental X $^2\Sigma^+$ well depth of 2.16_1 eV is in good agreement with the calculated values $D_e = 2.11_5 \text{ eV}$ (11) and $D_e = 2.15 \text{ eV}$ (14).

^bFrom the observation of Rydberg states in the absorption spectrum, and from ab initio calculations for BeH and BeH^+ ; see (12).

^c Λ -type doubling; for details see (13). R and P lines involving $v'=0$ and 1 are twice as broad as the corresponding Q lines. $v=2$ is strongly perturbed.

^d(13) suggest that the B and G states result from an avoided $^2\Pi - ^2\Pi$ crossing, the former (B $^2\Pi$) having a double minimum potential curve with a potential maximum corresponding to $T_e = 56950 \text{ cm}^{-1}$ at $r = 1.94 \text{ \AA}$.

$e_{\gamma_e} = -0.040$.

^fFor additional D_v and higher order constants see (13).

^gUsing isotope relations.

^hPerturbation at low N. Higher vibrational levels are probably predissociated.

ⁱLine width increases with decreasing N; the first lines are not observed.

^j(13) give 50888.57, without explanation. $A \approx 0$.

^k Λ -type doubling, $\Delta v_{ef}(v=0) = +0.217N(N+1)$.

^lThe B ↔ X bands ($v' \leq 2$, and fragments of the 3-3 band of Be^2H) consist of Q branches only except the 0-0 band which, in absorption, has P and R branches showing a marked broadening increasing with N. The predissociation mechanism involves both the unobserved $3p\sigma$ state and the first excited $^2\Sigma^+$ state which is unstable except at very large r

Be⁻H (continued):

values; for details see (15). The Q branch lines of Be¹H (Be²H) break off at N'=31, 24(38), 14(27), (14) in v'=0,1,2,3, respectively, owing to the presence of a maximum in the B²Π potential curve; see ^d. Two additional levels of Be¹H, very likely belonging to B²Π but called B'²Π(v', v'+1) in (13), are situated above the potential energy maximum in B²Π:

	T _e	B	D	
B' ² Π, v'+1	[58435.8]	6.01	187 × 10 ⁻⁴	} and higher or- der constants.
B' ² Π, v'	[58284.8]	8.34	129 × 10 ⁻⁴	

Transitions to these levels from X²Σ⁺ consist of Q branches only, breaking off at N'=14 in v'+1.

^my_e = -0.1324.

ⁿTaking into account the usually neglected contributions Y'₀₀ and Y''₀₀ to the zero point energies of A and X. A (spin-orbit) = +2.1; for an ab initio calc. see (4).

^oDerived (9) from pure vibronic energy separations which differ from the origins normally referred to in these tables.
^py_e = -0.47.

^qΛ-type doubling, Δv_{ef}(v=0) = +0.0141N(N+1) - ...; higher order constants in (9). Theoretical calculations (7)(8).

^ry_e = -0.0042.

^sHigher order constants in (9).

^tTheoretical absorption oscillator strengths (5)(6).

^uReversal of shading in some of the bands.

^vy_e = -0.38.

^wSpin splitting constant γ₀ = +0.005.

^xy_e = -0.0027.

^yβ_e = -0.039 × 10⁻⁴; higher order constants in (9).

^zIn Ar matrix at 4 K (10).

- (1) Watson, Parker, PR 37, 167 (1931).
- (2) Olsson, ZP 73, 732 (1932).
- (3) Watson, Humphreys, PR 52, 318 (1937).
- (4) Walker, Richards, PR 177, 100 (1969).
- (5) Henneker, Popkie, JCP 54, 1763 (1971).
- (6) Popkie, JCP 54, 4597 (1971).
- (7) Hinkley, Hall, Walker, Richards, JP B 5, 204 (1972).
- (8) Hinkley, Walker, Richards, JP B 5, 2016 (1972).
- (9) Horne, Colin, BSCB 81, 93 (1972).
- (10) Knight, Brom, Weltner, JCP 56, 1152 (1972).
- (11) Bagus, Moser, Goethals, Verhaegen, JCP 58, 1886 (1973).
- (12) Colin, De Greef, Goethals, Verhaegen, CPL 25, 70 (1974).
- (13) Colin, De Greef, CJP 53, 2142 (1975).
- (14) Meyer, Rosmus, JCP 63, 2356 (1975).
- (15) Lefebvre-Brion, Colin, JMS 65, 33 (1977).

BeF (continued):

- (12) Mishra, Khanna, IJPAP 7, 63 (1969).
- (13) Walker, Barrow, JP B 2, 102 (1969)

- (14) Walker, Richards, JP B 3, 271 (1970).
- (15) Rai, Singh, SpL 4, 129 (1971).
- (16) Farber, Srivastava, JCS FT I 70, 1581 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^9\text{Be}^2\text{H}$										
		$\mu = 1.64619882$	$D_0^0 = 2.06_6 \text{ eV}^a$						SEP 1976	
G 2_{II}	58750	302.5	Z 23.6	[2.747] ^{bc}		[10] ^d	[1.931]	G \leftarrow X, R	58134.9 Z	(3)
F 2_{Σ^+}	(56606)	(1598) ^e		[5.879]		[3.01] ^d	[1.319] ₈	F \leftarrow X,	56644.87 Z	(3)
E' (2_{Σ^+})	[54230.2] ^f			[5.260] ^f			[1.395] ₉ ^f	E' \leftarrow X,	50533.8 ^f Z	(3)
E 2_{Σ^+}	(54135)	(1460) ^e		[5.745] ^g		[3.8]	[1.335]	E \leftarrow X,	54104.9 Z	(3)
D $\left\{ \begin{array}{l} 2_{\Sigma^+} \\ 2_{II} \\ 2_{\Delta} \end{array} \right.$	(54000)	Strong absorption, complex structure.						D \leftarrow X,	54050	(3)
B 2_{II}	50906	1646.22	Z 25.15 ^h	5.9963 ^{ij}	0.1217 ^k	[3.114] ^d	1.3068	B \leftarrow X, V	50963.02 Z	(3)
A 2_{II_r}	20036.11 ^l	1551.13	Z 23.00	5.7614 ^m	0.1344 ⁿ	[3.181] ^o	1.3332	A \leftrightarrow X, V	20045.91 ^p Z	(1)* (2)
X 2_{Σ^+}	0	1530.32	Z 20.71	5.6872	0.1225 ^q	3.138 ^r	1.3419			
$^9\text{Be}^3\text{H}$										
		$\mu = 2.2597826_7$	$D_0^0 = 2.08 \text{ eV}^a$						APR 1976	
A 2_{II_r}	20037.91 ^b	1322 ^c	16 ^c	4.192	0.068 ^d	[1.66] ^e	1.334 ₀	A \rightarrow X, V	20045.83 ^f Z	(1)
X 2_{Σ^+}	0	1305 ^c	15 ^c	4.142	0.064 ^g	[1.67] ^e	1.342 ₀			
$^9\text{Be}^1\text{H}^+$										
				$D_0^0 = 3.14 \text{ eV}^a$						APR 1976
A 1_{Σ^+}	39417.0	1476.1	Z 14.8 ^b	7.184	0.125 ^c	6.1	1.608 ₉	A \rightarrow X, ^d R	39050.4 Z	(1)(3)
X 1_{Σ^+}	0	2221.7	Z 39.79 ^e	10.800	0.294 ^f	9.9	1.3122	Theoret. calc., pot. curves (4)(5)(6)		
$^9\text{Be}^2\text{H}^+$										
				$D_0^0 = 3.18 \text{ eV}^g$						APR 1976
A 1_{Σ^+}	39416.2	1096.4	Z 8.5	3.971	0.057 ₈	1.9	1.605 ₉	A \rightarrow X, R	39143.9 Z	(2)
X 1_{Σ^+}	0	1647.6	Z 21.9	5.955	0.123 ₃	2.9	1.3113			

Be²H: ^aFrom the value for Be¹H.
^bAverage from P,R and Q branches. Transitions to v'=1 and 2 consist of Q branches only, strongly perturbed for v'=2. The Q branch constants are given by $B'_v = 2.197 + 1.205(v+\frac{1}{2}) - 0.167(v+\frac{1}{2})^2$.
^cSee ^d of Be¹H.
^dAdditional D_v and higher order constants in (3).
^eUsing isotope relations.
^fUnidentified single level, vibrational numbering unknown. In absorption from v''=2.
^gSee ⁱ of Be¹H.
^hInclusion of v=3 changes these constants to $\omega_e = 1607.29$, $\omega_e x_e = -5.32$, $\omega_e y_e = -6.77$.
ⁱ Λ -type doubling, $\Delta v_{ef}(v=0) = +0.074 \times N(N+1)$.
^jSee ^d and ^l of Be¹H.
^k $\gamma_e = -0.0089$ ($v \leq 2$); recalculated from (3).
^lSee ⁿ of Be¹H. $A \approx +1.9$.
^m Λ -type doubling, $\Delta v_{ef}(v=0) = +0.00419 \times N(N+1) - \dots$; additional constants in (2).
ⁿ $\gamma_e = -0.0003$.
^oFor additional D_v and higher order constants see (2).
^pPure vibronic energy difference, not to be confused with the band origin as usually defined in these tables. See (2).
^q $\gamma_e = -0.001$.
^r $\beta_e = -0.022 \times 10^{-4}$; higher order constants in (2).
(1) Koontz, PR 48, 707 (1935).
(2) See ref. (9) of Be¹H.
(3) See ref. (13) of Be¹H.

Be³H: ^aFrom the value for Be¹H.
^bSee ⁿ of Be¹H.
^cFrom isotope relations. $\omega'_e - \omega''_e = 16.36$, $\omega'_e x'_e - \omega''_e x''_e = 0.84$, $\omega'_e y'_e - \omega''_e y''_e = -0.15$.
^d $\gamma_e = -0.007$.
^eAdditional D_v and higher order constants in (1).
^fSee P of Be²H.
^g $\gamma_e = -0.006$.
(1) De Greef, Colin, JMS 53, 455 (1974).
Be¹H⁺, Be²H⁺:
^aD₀⁰(Be¹H) + I.P.(Be) - I.P.(Be¹H).
^b $\omega_e y_e = -0.38$; -0.038 in (3) is obviously wrong.
^c $\gamma_e = -0.0054$.
^dTheoretical oscillator strength (7).
^e $\omega_e y_e = -0.21$; -0.021 in (3) is obviously wrong.
^f $\gamma_e = -0.0049$.
^gFrom the value for Be¹H⁺.
(1) Bengtsson-Knave, NARSSU (IV) 8, No. 4, 65 (1932).
(2) See ref. (1) of Be²H.
(3) See ref. (3) of Be¹H.
(4) Reed, Vanderslice, Jenč, JCP 37, 205 (1962).
(5) Brown, JCP 51, 2879 (1969).
(6) Banyard, Taylor, JP B 8, L137 (1975).
(7) Stewart, Watson, Dalgarno, JCP 63, 3222 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^9\text{Be}^{127}\text{I}$		$\mu = 8.4146148$								SEP 1976
A $\begin{cases} 2\Pi_{3/2} \\ 2\Pi_{1/2} \end{cases}$	23544.7	603.8	H	2.1	$[0.4182]$ $[0.4216]^a$	$[0.80]$ $[0.73]$	$[2.188_7]$ $[2.179_9]$	A \rightarrow X, R	23900.83 Z 23540.59 Z	(1)* (2)
X $2\Sigma^+$	0	611.7	H	1.6	$[0.4219]^b$	$[0.82]$	$[2.179_1]$			
$^9\text{Be}^{(84)}\text{Kr}^+$		$(\mu = 8.1376909)^a$								APR 1976 A
A 2Π	23857 23692	557	H	3.5				A \rightarrow X, V	23954 23789	H H (1)*
X $2\Sigma^+$	0	364	H	5.4						
$^9\text{Be}^{16}\text{O}$		$\mu = 5.7643273_5$ $D_0^0 = 4.6_0 \text{ eV}^a$								APR 1976
		Fragments of additional singlet and triplet systems in the region 29000 - 33000 cm^{-1} .								(1)(4)(10)*
C $(^1\Sigma)$	39120.2	1081.5 (H ^Q)	9.1	(1.308)	(0.010)		(1.495)	C \rightarrow A, ^b R	29683.1 (H ^Q)	(5)(10)*
B $1\Sigma^+$	21253.94	1370.82 Z	7.746 ^c	1.5758 ^{de}	0.0154	8.41 ^f	1.3623	B \rightarrow A, ^g V	11961.78 Z	(10)
b $3\Sigma^+$	j							B ^h \leftrightarrow X, ⁱ R	21196.70 Z	(1)(2)(7) (10)(13)* (16)
A 1Π	9405.61	1144.24 Z	8.415 ^k	1.3661 ^{lde}	0.01628 ^m	7.79 ⁿ	1.4631	A \rightarrow X, R	9234.92 Z	(3)(6)* (9) (10)*
a 3Π	(8480) ^o							For computed ground state properties see (17)(24).		
X $1\Sigma^+$	0	1487.32 Z	11.830 ^p	1.6510 ^e	0.0190	8.20 ^q	1.3309			

BeI: ^a Λ -type doubling, $\Delta v_{fe} = +0.0938(\text{J} + \frac{1}{2})$.

^bSpin splitting constant $\gamma_0 = +0.0459$.

(1) Murty, Rao, CS 38, 187 (1969); PRIA A 72, 71 (1972).

(2) Carleer, Colin, to be published.

BeKr⁺: ^aReduced mass of Be⁺ + Kr.

(1) Subbaram, Coxon, Jones, CJP 53, 2016 (1975).

BeO: ^aThermochemical value (mass-spectrom.)(14); in good agreement with 4.52 eV derived from an ab initio calculation (24) of $X^1\Sigma^+$. Extrapolations of X and A to their common limit $Be(^1S) + O(^1D)$ lead to 3.9 and 4.8₂ eV, respectively (12). A considerably higher thermochemical value of 5.5₁ eV was determined by (11).

^bFranck-Condon factors (22).

^c $w_e y_e = -0.00027$.

^dNumerous perturbations between levels of $A^1\Pi$ and $B^1\Sigma$, $A^1\Pi$ and $X^1\Sigma$, as well as perturbations by unidentified levels [probably belonging to a $^3\Pi$ and $b^3\Sigma$, see (20)]. For an extensive treatment see (6)(7)(8)(10).

^eRKR potential curves (21).

^f $\beta_e = -0.07 \times 10^{-6}$; $H_v = +[27 - 2(v + \frac{1}{2})] \times 10^{-12}$.

^gVery weak system.

^hRadiative lifetime $\tau(v=0) = 90$ ns (25); $f_{00} = 0.0335$. A much smaller value, $f_{00}(B-X) = 0.00194$, was estimated from shock tube measurements (19).

ⁱFranck-Condon factors (15)(22); approximate electronic transition moments, band oscillator strengths (19).

^jThe theoretical calculations of (18) place the $^3\Sigma^+$ state at 4100 cm^{-1} below $B^1\Sigma^+$, in rough agreement with (23) who calculate its energy at 15400 cm^{-1} above $X^1\Sigma$.

^k $w_e y_e = +0.0339$.

^l Λ -type doubling, $\Delta v_{fe} = +0.00055 J(J+1)$.

^m $y_e = +0.000055$.

ⁿ $\beta_e = -0.044 \times 10^{-6}$.

^oTheoretical calculations (20)(18) place the $^3\Pi$ state at 920 to 2600 cm^{-1} below $A^1\Pi$, in reasonable agreement with (26) who predict it at 5900 cm^{-1} above $X^1\Sigma^+$.

^p $w_e y_e = +0.0224$.

^q $\beta_e \approx -0.01$; $H_v = +[12.5 - 1.1(v + \frac{1}{2})] \times 10^{-12}$.

BeO (continued):

- (1) Bengtsson, AMAF A 20, No. 28 (1928).
- (2) Rosenthal, Jenkins, PR 33, 163 (1929).
- (3) Herzberg, ZP 84, 571 (1933).
- (4) Ciccone, RiSc (VI) 2, 3 (1935).
- (5) Harvey, Bell, PPS 47, 415 (1935).
- (6) Lagerqvist, Westöö, AMAF A 31, No. 21 (1945).
- (7) Lagerqvist, Westöö, AMAF A 32, No. 10 (1945).
- (8) Lagerqvist, AMAF A 33, No. 8 (1946).
- (9) Lagerqvist, AMAF B 34, No. 23 (1947).
- (10) Lagerqvist, Dissertation (Stockholm, 1948).
- (11) Drummond, Barrow, TFS 49, 599 (1953).
- (12) Lagerqvist, AF 7, 473 (1954).
- (13) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (14) Chupka, Berkowitz, Giese, JCP 30, 827 (1959).
- (15) Nicholls, Fraser, Jarman, McEachran, ApJ 131, 399 (1960).
- (16) Thrush, PCS (1960), p. 339.
- (17) Yoshimine, JCP 40, 2970 (1964); JPSJ 25, 1100 (1968).
- (18) Verhaegen, Richards, JCP 45, 1828 (1966).
- (19) Drake, Tyte, Nicholls, JQSRT 7, 639 (1967).
- (20) Huo, Freed, Klemperer, JCP 46, 3556 (1967).
- (21) Thakur, Singh, JSRBHU 18, 253 (1968).
- (22) Liszt, Smith, JQSRT 11, 1043 (1971).
- (23) O'Neil, Pearson, Schaefer, CPL 10, 404 (1971).
- (24) Schaefer, JCP 55, 176 (1971).
- (25) Capelle, Johnson, Broida, JCP 56, 6264 (1972).
- (26) Pearson, O'Neil, Schaefer, JCP 56, 3938 (1972).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^9\text{Be}^{32}\text{S}$		$\mu = 7.0304599$ $D_0^0 = 3.8 \text{ eV}^a$								APR 1976
b ($^3\Pi$)								(b \leftarrow a), R	$\begin{Bmatrix} 25961.8 & \text{H} \\ 25941.8 & \text{H} \\ 25924.5 & \text{H} \end{Bmatrix}$	(2)*
B $^1\Sigma^+$	25941.6	851.35	Z	4.85	0.72894	0.00604 ^b	2.14	B \leftrightarrow X, R	25868.61 Z	(1)(2)*
C ($^1\Delta$)	[13545.8] ^c	[660.7] ^c		5.5	[0.5963] ^c	0.0069				
A $^1\Pi$	7960.1	762.46 ^d	Z	4.12	0.6590 ^{def}	0.00605 ^g	2.00	A \rightarrow X, R	7842.9 ^d Z	(2)
a ($^3\Pi$)										
X $^1\Sigma^+$	0 ^h	997.94	Z	6.137	0.79059	0.00664 ⁱ	2.00		1.7415 ₃	
$^9\text{Be}^{(132)}\text{Xe}^+$		$(\mu = 8.4353358)^a$								APR 1976
A $^2\Pi$	22273 21922	545	H	3.9				A \rightarrow X, V	22360 22009	(1)*
X $^2\Sigma^+$	0	371	H	3.7						
$^{11}\text{B}^{19}\text{F}$		$\mu = 6.9701832_5$ $D_0^0 = 7.8_1 \text{ eV}^a$ I.P. = 11.115 eV ^b								APR 1976
		Rydberg series (abs.) beginning with D, J, P, ... : $\begin{Bmatrix} \nu(1-0) = 91330 \\ \nu(0-0) = 89650 \end{Bmatrix}$						$- R/(n-0.52)^2 \begin{Bmatrix} n \leq 18. \\ n \leq 15. \end{Bmatrix}$		(24)*
		Rydberg series (abs.) beginning with C, I, O, ... : $\begin{Bmatrix} \nu(1-0) = 91330 \\ \nu(0-0) = 89650 \end{Bmatrix}$						$- R/(n-0.66)^2, n \leq 9.$		(24)
R $^1\Sigma^+(6s\sigma)^c$	[85848]							R \leftarrow X, V	85150	H (24)
P $^1\Pi(5p\pi)$	84077	[1673]	H ^Q		[1.651 ₁] ^d		[6.4] ^d	P \leftarrow X, V	84215	H ^Q (24)
O $^1\Sigma^+(5p\sigma)$	83680.2	1676	H	9.5	[1.6275]		[5.6]	O \leftarrow X, V	83817.71 Z	(24)
L $^1\Sigma^+(5s\sigma)$	[83348.32]				[1.5578]		[-21.3]	L \leftarrow X, V	82650.21 Z	(24)
J $^1\Pi(4p\pi)$	80544	[1673.0 ₉]	Z		1.6516 ^e	0.0162	[6.5]	J \leftarrow X, V	80681.98 Z	(24)
h $^3\Pi$	80230	[1679.2]	H ^Q		[1.647 ₅] ^f		[6.2]	h \rightarrow b, V	19225.28 Z	(24)
I $^1\Sigma^+(4p\sigma)$	79631.3 ₉	1666.28	Z	12.57	1.6382	0.0174	[6.4]	I \leftarrow X, V	79763.28 Z	(24)
H $^1\Sigma^+(3d\sigma)$	[79389.3 ₂]				[1.6511]		[13.0]	H \leftarrow X, V	78691.2 ₁ Z	(24)

BeS: ^aFrom Gaydon (4).

^b $r_e = -0.00003$.

^cConstants for the lowest observed level and interval, vibrational numbering unknown. From perturbations in A ¹ Π .

^dVibrational numbering uncertain.

^eConstants for the f component; $\Delta v_{fe} \approx +0.00015 \times J(J+1)$.

^fThe A ¹ Π state is perturbed by three states, one of them being X ¹ Σ^+ , another probably ¹ Δ .

^g $r_e = +0.000025$.

^hTheoretical calculations (3) support a ¹ Σ ground state.

ⁱ $r_e = -0.00002$.

(1) Gissane, Barrow, PPS 82, 1065 (1963).

(2) Cheetham, Gissane, Barrow, TFS 61, 1308 (1965).

(3) Verhaegen, Richards, PPS 90, 579 (1967).

(4) Gaydon, DISSEN (1968).

BeXe⁺: ^aReduced mass of Be⁺ + Xe.

(1) Coxon, Jones, Subbaram, CJP 53, 2321 (1975).

BF: ^aThermochemical value (mass-spectrom.)(15)(18). Extrapolation of A ¹ Π gives 8.0₂ eV (9).

^bExtrapolation of Rydberg series; 11.06 eV by electron impact (26).

^cApproximate description of the Rydberg electron (24); see also (17).

^dComputed from the data for ¹⁰B¹⁹F; $B_0 = 1.7551$, $D_0 = 7.2 \times 10^{-6}$, $\Delta v_{ef} = +0.0146 \times J(J+1)$.

^e $\Delta v_{ef} = +0.0056 \times J(J+1) - \dots$

^f $\Delta v_{ef} = +0.0024 \times N(N+1)$.

(continued p. 87)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
¹¹ B ¹⁹ F (continued)										
g $^3\Sigma^+$ [78771.9] F $^1\Pi$ (3d π) (77406)		(1670) ^h		[1.676 ₅] [1.672 ₃] ^{i,j}		[5.1] [8.9]	[1.201 ₁] [1.202 ₆]	g \rightarrow b, ^g V 16927.59 Z F \rightarrow A, V 26454.1 ₃	(24) (12)*	
f $^3\Pi$ 77405		[1678.1] Z		[1.641 ₇] ^k		[5.0]	[1.213 ₈]	F \leftarrow X, V 77542.7 ₉ Z f \rightarrow c, V 10428.15 Z f \rightarrow b, V 16400.10 Z	(24) (24)* (24)	
G $^1\Sigma^+$ (4s σ) 76952		[1685.63] Z		1.6054	0.0147	[1.2] ^l	1.2274	G \rightarrow B, R 11596.99 G \leftrightarrow X, V 77096.41 Z	(12)* (10)(24)*	
E $^1\Delta$ (3d δ) (76292) e $^3\Sigma^+$ 75916		(1581) ^h [1654.29] Z		[1.6209] ^m 1.6447		[6.4] [6.3]	[1.2215] 1.2126	E \rightarrow A, V 25295.69 Z e \rightarrow b, ^g 14899.56 Z	(12)* (24)* (12)* (22) (24)*	
D $^1\Pi$ (3p π) 72144.4 ₂		[1661.96] Z	11.7 H ^Q	1.6282 ⁿ	0.0170	[6.3]	1.2188	D \leftrightarrow X, V 72286.06 Z	(4)(5)(10) (24)*	
d $^3\Pi$ 70710.4 C $^1\Sigma^+$ (3p σ) 69030.3 ₈		1696.71 Z 1613.1 ₀ Z	11.01 14.5 ₀	1.6517 ^{op} 1.6238	0.0176 ^q 0.0194	[6.5] [7.3]	1.2101 1.2204	d \rightarrow b, 9711.65 Z C \rightarrow A, V 18046.53 C \leftrightarrow X, V 69135.19 Z	(24)* (12)* (4)(5)* (10) (24)	
c $^3\Sigma^+$ 67045 B $^1\Sigma^+$ (3s σ) 65353.9 ₃		[1541.3] Z 1693.5 ₁ Z		[1.603 ₀] ^r 1.6590		[5.5] ^r [7.6]	[1.228 ₃] 1.2074	c \rightarrow a, V 38011.97 Z B \rightarrow A, V 14410.76 B \leftrightarrow X, V 65499.42 Z	(2)(8)(16) (12)* (4)(5)* (10) (24)	
b $^3\Sigma^+$ 61035.3		1629.28 Z	22.25 ₅	1.6385	0.0200 ^s	[7.0]	1.2149	b \rightarrow a, ^t V 32040.42 Z	(1)(2)(3)* (6)(8)(16)	
A $^1\Pi$ 51157.45		1264.9 ₆ Z	12.5 ₃ ^u	1.4227 ^v	0.0180 ^w	[7.3]	1.3038	A ^x \leftrightarrow X, ^y R 51088.66 Z	(4)(5)* (7) (11)* (24)	
a $^3\Pi_r$ 29144.3 ^z		1323.8 ₆ Z	9.20 ^{a'}	1.413 ₅ ^{b'}	0.0158	[6.3]	1.308 ₁	a \rightarrow X, R 29105.8 Z	(28)	
X $^1\Sigma^+$ 0		1402.1 ₃ Z	11.8 ₄ ^{c'}	[1.507235]	0.0198	[7.6]	1.2625 ₉	Microwave sp. ^{d'}	(27)	

BF (continued):

- ^eHeadless band.
^hEstimated from observed isotope shifts.
ⁱ $\Delta v_{ef} = + 0.0423 \times J(J+1) - \dots$
^jLines with $J' \leq 6$ are weak or absent, both in emission and in absorption.
^k $\Delta v_{ef} = - 0.0289 \times N(N+1) + \dots$
^l $D_1 = 22.8 \times 10^{-6}$.
^m $\Delta v_{ef} \approx - 4 \times 10^{-7} J^2(J+1)^2$.
ⁿ $\Delta v_{ef} = + 0.0009 \times J(J+1)$.
^o $\Delta v_{ef} = + 0.0011 \times N(N+1)$.
^pThe emission from $v=4$ consists of Q branch lines only.
^q $\gamma_e = + 0.0002$.
^rFrom (24). Barrow et al. (8) give $B_0 = 1.605_2$, $D_0 = 8.2 \times 10^{-6}$.
^s $\gamma_e = - 0.0012$.
^tFranck-Condon factors (21).
^u $w_{ey_e} = - 0.24_2$. This state may have a potential hump of $\sim 0.2_2$ eV.
^v $\Delta v_{ef} \approx - 0.0002 \times J(J+1)$.
^w $\gamma_e = - 0.00040$.
^xRadiative lifetime $\tau(v=0,1,2) = 2.8$ ns; $f_{00} = 0.40$ (20)(23).
^yFranck-Condon factors (25).
^z $A = + 24.2_5$.
^a $w_{ey_e} = + 0.047$.
^b Λ -type doubling; see (8).
^c $w_{ey_e} = + 0.05_6$.
^d $\mu_{el}(v=0) = 0.5$ D. Values of $eqQ(^{10,11}B)$ in (27). For computed ground state properties see (13)(14)(19).

- (1) Dull, PR 47, 458 (1935).
(2) Strong, Knauss, PR 49, 740 (1936).
(3) Paul, Knauss, PR 54, 1072 (1938).
(4) Chrétien, Miescher, Nature 163, 996 (1949); HPA 22, 588 (1949).
(5) Chrétien, HPA 23, 259 (1950).
(6) Dodsworth, Barrow, PPS A 68, 824 (1955).
(7) Onaka, JCP 27, 374 (1957).
(8) Barrow, Premaswarup, Winternitz, Zeeman, PPS 71, 61 (1958).
(9) Barrow, TFS 56, 952 (1960).
(10) Mal'tsev, OS(Engl. Transl.) 2, 225 (1960).
(11) Verma, CJP 39, 1377 (1961); 40, 1852 (1962)[Erratum].
(12) Robinson, JMS 11, 275 (1963).
(13) Nesbet, JCP 40, 3619 (1964); 43, 4403 (1965).
(14) Huo, JCP 43, 624 (1965).
(15) Hildenbrand, Murad, JCP 43, 1400 (1965).
(16) Krishnamachari, Singh, CS 34, 655 (1965).
(17) Lefebvre-Brion, Moser, JMS 15, 211 (1965).
(18) Murad, Hildenbrand, Main, JCP 45, 263 (1966).
(19) Hegstrom, Lipscomb, JCP 45, 2378 (1966); 48, 809 (1968).
(20) Hesser, Dressler, JCP 45, 3149 (1966).
(21) Pathak, Maheshwari, IJPAP 5, 138 (1967).
(22) Czarny, Felenbok, CPL 2, 533 (1968).
(23) Hesser, JCP 48, 2518 (1968).
(24) Caton, Douglas, CJP 48, 432 (1970).
(25) Wentink, Spindler, JQSRT 10, 609 (1970).
(26) Hildenbrand, IJMSIP 7, 255 (1971).
(27) Lovas, Johnson, JCP 55, 41 (1971).
(28) Lebreton, Ferran, Marsigny, JP B 8, L465 (1975).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻³ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	v ₀₀	
<div>"B'H</div> <div>μ = 0.92330324 D₀⁰ = 3.42 eV^a I.P. = 9.77 eV^b</div> <div>Fragments in the region 74420 - 74523 cm⁻¹.</div> <div>Fragments only.</div> <div>" " .</div> <div>APR 1976 A</div>										
(5d)								5d ← X,		(7)
K 1Π (4d)								K ← X,	71840	(7)
J 1Σ ⁺ (4p)								J ← X,	70040	(7)
I 1Σ ⁺ 4s				[11.99] ^c			[1.234]	I ← X, ^d	67395.8 Z	(7)(22)
H 1Δ } 3d				[12.25 ₅] ^c			[1.220 ₆]	H ← A,	43345.7 Z	(7)* (22)
G 1Π }								H ← X,	66419.7 Z	
F 1Σ ⁺ }								G ← X,	66399.3 Z	
E 1Σ ⁺ } 3p				[12.32 ₁]		[1.3]	[1.217 ₃]	F ← X,	66079.5 Z	(7)*
D 1Π }								E ← X,	61872.3 Z	
C 1Σ ⁺	55281.1	2474.7 ₂	Z 54.42 ₄ ^e	12.410 ^f	0.432	[1.24 ₇] ^g	1.2129	D ← X,	61105.4 Z	
B 1Σ ⁺ 3s	52335.8	2399.9 ₁	Z 69.51 ₉ ^h	12.339 ⁱ	0.485 ^j	1.26 ^k	1.2164	C → A, V	32259.7 ₈ Z	(4)(13)
c 3Σ ⁺ l								C ← X, ^d	55333.6 ₉ Z	(7)
C' 1Δ	45981.0	2610.0 ₂	Z 46.6 ₂	12.757	0.390	1.219 ^m	1.1963	B → A, V	29272.7 ₃ Z	(4)
b 3Σ(-)				[12.126]		[1.28]	[1.2271]	B ← X, ^d	52346.6 ₉ Z	(7)* (13)
A 1Π	23135.8	2250.9 ₉	Z 56.66 ₅ ⁿ	12.295 ₂ ^{opq}	0.834 ₆ ^r	[1.451] ^g	1.2186	C' ↔ A, V	23029.2 ₁ Z	(13)*
a 3Π t				[12.667] ^u		[1.22]	[1.2006]	b → a, R	27060.8 Z	(1)(2)
X 1Σ ⁺ 0		2366.9 ₀	Z 49.39 ₅ ^v	12.021 ^w	0.412	1.242 ^x	1.2324	A ^s ↔ X, R _v	23073.9 ₆ Z	(1)* (2)(5) (13)*
Summary of theoretical calculations: see ref. in (12)(14)(20)(23).										

B¹H: ^aFrom the predissociation by rotation in A ¹Π (13); see P. The estimated height (see ⁿ) of the potential hump in A ¹Π was subtracted from the extrapolated energy of the potential maximum. Good agreement with theory [(9), additional results summarized in (23)].

^bFrom the observation of Rydberg states in the absorption spectrum (7); theoretical computations (21) give 9.53 eV.

^cThe rotational constants for the 4s state and the 3d complex were re-determined by Johns and Lepard (22) using a model which gives proper consideration to the effects of s~d mixing. Ginter (10) obtained effective constants for the four states involved.

^dNearly undegraded, headless band.

^e $w_e y_e = + 0.22_8$.

^fPredissociation in v=2 for J>8. v=3 perturbed at low J.

^gAdditional D_v and higher order constants in (13).

^h $w_e y_e = - 3.92_7$.

ⁱTheoretical calculations (16)(18) predict a double minimum potential curve.

^j $r_e = - 0.042_4$.

^k $\beta_e = + 0.10 \times 10^{-3}$; $H_0 = + 0.56 \times 10^{-9}$.

^lThe lowest ³Σ⁺ state, T_e ≈ 51700 (11)(18), is predicted (18) to be Rydberg-like (3sδ) and quasi-bound at small internuclear distances, but valence-like and repulsive (dissociating into ground state atoms) for separations larger than 1.45 Å.

^m $\beta_e = - 0.020 \times 10^{-3}$; $H_e \approx 1.00 \times 10^{-7}$.

ⁿ $w_e y_e = - 15.83_0$. This state has a potential hump (3)(13) of approximately 0.155 eV (6)(19).

^oΛ-type doubling, Δv_{ef} = + [0.0389 - 0.0027(v+½)]J(J+1).

^pPredissociation by rotation. J' of the first missing or first diffuse lines:

	v'=0	1	2	3
em./abs.:	27/30	21/24	14/17	-/6

^q $\mu_{el}(v=0) = 0.58 D (15)$.

^r+ 0.132₂(v+½)² - 0.05188(v+½)³.

^sRadiative lifetime τ = 159 ns; f₀₀ = 0.035 (17).

^tA₀ = + 5.95. Theoretical estimates of T_e range from 2800 to 9700 cm⁻¹; see the summary in (14), also (19).

^uΛ-type doubling; see (2).

^v $w_e y_e = + 0.36_4$.

^w $\mu_{el}(v=0) = 1.2_7 D (15)$. Theory (8) predicts a large negative rotational magnetic moment of - 8.27 μ_N.

^x $\beta_e = - 0.026 \times 10^{-3}$. Higher order constants in (13).

- (1) Lochte-Holtgreven, van der Vleugel, ZP 70, 188 (1931).
- (2) Almy, Horsfall, PR 51, 491 (1937).
- (3) Herzberg, Mundie, JCP 8, 263 (1940).
- (4) Douglas, CJR A 19, 27 (1941).
- (5) Thrush, Nature 186, 1044 (1960).
- (6) Hurley, PRS A 261, 237 (1961).
- (7) Bauer, Herzberg, Johns, JMS 13, 256 (1964).
- (8) Stevens, Lipscomb, JCP 42, 3666 (1965); ref. (19) of BF.
- (9) Ellison, JCP 43, 3654 (1965).
- (10) Ginter, JCP 44, 950 (1966).
- (11) Grimaldi, Lecourt, Lefebvre-Brion, Moser, JMS 20, 341 (1966).
- (12) Cade, Huo, JCP 47, 614 (1967).
- (13) Johns, Grimm, Porter, JMS 22, 435 (1967).
- (14) Harrison, Allen, JMS 29, 432 (1969).
- (15) Thomson, Dalby, CJP 47, 1155 (1969).
- (16) Browne, Greenawalt, CPL 7, 363 (1970).
- (17) Smith, JCP 54, 1384 (1971).
- (18) Pearson, Bender, Schaefer, JCP 55, 5235 (1971).
- (19) Blint, Goddard, CP 3, 297 (1974).
- (20) Banyard, Taylor, JP B 8, L137 (1975).
- (21) Griffing, Simons, JCP 62, 535 (1975).
- (22) Johns, Lepard, JMS 55, 374 (1975).
- (23) Meyer, Rosmus, JCP 63, 2356 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-3}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{11}\text{B}^2\text{H}$											
		$\mu = 1.70261633$		$D_0^0 = 3.46 \text{ eV}^a$						APR 1976	
H 1Δ	3d			[6.63 ₅]			[1.221 ₆]	H \leftarrow X,	66448.0 Z	}(2)*	
G 1Π								G \leftarrow X,	66362.8 Z		
F $1\Sigma^+$								F \leftarrow X,	66068.6 Z		
E $1\Sigma^+$	3p			[6.73 ₆]		[0.4]	[1.212 ₄]	E \leftarrow X,	61852.8 Z	}(2)*	
D 1Π								D \leftarrow X,	61110.2 Z		
B $1\Sigma^+$	3s	52348 ^b	[1700.3 ₄]	Z 46.6	6.70 ₅	0.19 ₅ ^c	0.4 ^d	1.215 ₂	B \leftarrow X, ^e	52360.2 ₁ Z	(2)*
A 1Π	23142		[1594.0 ₈]	Z (43)	6.648 ^f	0.280	0.403 ^g	1.220 ₄	A \rightarrow X, ν_R	23098.75 Z	(1)(2)
X $1\Sigma^+$	0		[1703.2 ₆]	Z (28)	6.54 ₂	0.17 ₁	0.4 ₂ ^h	1.230 ₂			
$^{11}\text{B}^1\text{H}^+$											
				$D_0^0 = 1.95 \text{ eV}^a$						APR 1976	
A $2\Pi_r$	b			[11.565] ^c		[1.24]	[1.2565]	A \rightarrow X, R	26376.2 Z	(1)	
X $2\Sigma^+$	0			[12.374]		[1.25] ^d	[1.2147]				
$(^{11})\text{B}^{127}\text{I} ?$											
		$(\mu = 10.1304606)$								APR 1976	
				Absorption bands in the region 35870 - 37590 cm^{-1} have been attributed (1) to BI, but are almost certainly due to BCl (A \leftarrow X).							

B^2H : ^aFrom the value for B^1H .
 ^bLarge electronic isotope shift; see (3).
 ^c $\gamma_e = -0.014$.
 ^d $H_0 = +0.35 \times 10^{-9}$.
 ^eHeadless bands.
 ^fThunberg's (1) value of 6.653 was derived from R and P
 branches only; $\Delta v_{ef} = +0.0102 \times J(J+1)$.
 ^g $\beta_e = +0.034 \times 10^{-3}$.
 ^h $\beta_e = -0.05 \times 10^{-3}$.

 (1) Thunberg, ZP 100, 471 (1936).
 (2) See ref. (7) of B^1H .
 (3) Bunker, JMS 28, 422 (1968).

B^1H^+ : ^a $D_0^0(B^1H) + I.P.(B) - I.P.(B^1H)$.
 ^b $A = +14.0$.
 ^c Λ -type doubling, $\Delta v_{ef} \approx +0.0164 \times N(N+1) - \dots$.
 ^d $H_0 = +6.9 \times 10^{-8}$.
 (1) See ref. (2) of B^1H .

 BI: (1) Briggs, Piercy, SA A 29, 851 (1973).

State ^a	T _e	ω _e		ω _e x _e	B _e	α _e	D _e (10 ⁻⁹ cm ⁻¹)	r _e (Å)	Observed Transitions		References
									Design.	ν ₀₀	
²⁰⁹ Bi ₂											
μ = 104.490201 D ₀ ⁰ = 2.0 ₄ eV ^b											
y	x + 15746.3	94.7	H	5.2					y → x, R	15741.4	H (9)
x	x	103.2	H	2.45							
Fragments of several absorption systems in the region 44800 - 52900 cm ⁻¹ .											
D	(42228) ^c	129	H	9.7					D ← (A) ^c , R	24485	H (1)*
Three diffuse absorption bands at 40115, 40275, 40467 cm ⁻¹ .											
C	36456	155.2 ^d	H	2.3 ^e					C ← X, R	36447	H (1)* (2)
I	33216.7	156.4	H	6.1					I → A, V	15487.9	H (8)*
H	[32657.1]	Only ν' = 0.							H → A, V	14851.6	H (8)*
Continuous absorption with maximum at 32000 cm ⁻¹ .											
G	(29609.0) ^f	107.0 ^f	H	0.2					G → (A) ^f , R	11857.0	H (8)*
E	(26504.7)	(63.5) ^g		(8.5)	(0.01425) ^g	(0.00015)			E → B, 21470.9 ^h (Z)		(11)
A	0 _u ⁺ 17739.3	132.49	H	0.302 ⁱ	0.01968 ^{jk}	0.000053	ℓ	2.863	A ↔ X, R	17719.2	H (1)* (2)(4) (8)* (11)
A'	(8000) ^m	141.2		0.37 ⁿ							
B	(5000) ^m	127.0 ₅		0.29 ^o	(0.01790)	(0.000046)					
X	1Σ _g ⁺ 0 ^m	172.71	H	0.341 ^p	[0.022781] ^k	0.000055 ^q	[1.50]	2.6596			
X'	(-1500) ^m	154.3		0.42							

Bi₂: ^aThe state designations adopted in the Bi₂ table agree with those of (11). They are compared below with designations used elsewhere:

This table, and (11):	X'	X	B	A'	A	E	G	H	I	C	D
(1):		A			B					C	D
(3):		X			B					D	E
(4):		X			A						
(7):		X			A					C	D
(8):		X			A		G	H	I	D	E

Bi₂ (continued):

- ^bThermochemical value (mass-spectrom.)(5)(6), calculated for a ¹Σ ground state and disregarding other low-lying states.
- ^cContrary to the conclusion of Almy and Sparks (1) that the violet system involves low vibrational levels of A, Gerber and Broida (11) consider it more probable that the absorption originates in high vibrational levels ($v'' \approx 20$) of X', thereby reducing T_e to approximately 26000 cm⁻¹. Additional unassigned diffuse absorption features in the region 22000 - 24000 cm⁻¹.
- ^d(2) give $\omega_e = 146.0$, $\omega_e x_e = 0.50$. All bands except those with $v' = 1$ are diffuse. Observed to $v' = 4$. At shorter wavelengths are additional features probably belonging to C←X but not assigned by (1).
- ^eThe value of $\omega_e x_e$ given by (1) is clearly $2\omega_e x_e$. The constants listed above take account of this correction.
- ^fGerber et al. (11) have found very similar constants ($\omega_e = 105.68$, $\omega_e x_e = 0.63$) for the lower state of an unidentified transition in the laser photoluminescence spectrum and have tentatively identified this lower state with the upper state of Reddy and Ali's (8) G→A system. They suggest that the emission from G involves high vibrational levels ($v'' \approx 50$) of X, rather than $v=0, \dots, 4$ of A, and they estimate $T_e \approx 20000$.
- ^gConstants derived from intensity data; see (11).
- ^hRecalculated from data in (11).
- ⁱ $\omega_e y_e = -0.0021$, $\omega_e z_e = +0.000055$ (8). Slightly different constants in (1)(11).
- ^jExtrapolated from B₈, B₉, B₁₁ (4).
- ^kRKR potential curves (7a)(11).
- ^l $D_8 = 1.71 \times 10^{-9}$.

^mAll four states give rise to long lower state progressions in the laser photoluminescence spectrum of Bi₂ (11). Their relative energies were estimated (11) from the temperature dependence of the photoluminescence intensities. The upper levels of the transitions, except those belonging to A and E, could not be identified.

$${}^n\omega_e y_e = -0.0019.$$

$${}^o\omega_e y_e = -0.001.$$

$${}^p\omega_e y_e = -0.0018, \omega_e z_e = +0.00001_0 \text{ (8). Slightly different constants in (1)(11).}$$

^qFrom the laser photoluminescence spectrum (11), adjusted for best overall fit of observed with calculated intensities.

- (1) Almy, Sparks, PR 44, 365 (1933).
- (2) Nakamura, Shidei, JJP 10, 11 (1935).
- (3) Herzberg, MOLSPEC 1 (1950).
- (4) Åslund, Barrow, Richards, Travis, AF 30, 171 (1965).
- (5) Kohl, Uy, Carlson, JCP 47, 2667 (1967).
- (6) Rovner, Drowart, Drowart, TFS 63, 2906 (1967).
- (7) DONNSPEC (1970).
- (7a) Rao, Lakshman, IJPAP 8, 785 (1970).
- (8) Reddy, Ali, JMS 35, 285 (1970).
- (9) Singh, Nair, Rai, SpL 4, 313 (1971).
- (10) Topouzkhanian, Sibaï, d'Incan, ZN 29 a, 436 (1974).
- (11) Gerber, Sakurai, Broida, JCP 64, 3410 (1976); Gerber, Broida, JCP 64, 3423 (1976).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{209}\text{Bi}^{79}\text{Br}$		$\mu = 57.285367_3$ Fragments of three systems of V shaded absorption bands in the regions 40800 - 45000 and 33700 - 36900 cm^{-1} .								MAY 1976
B	24710.9	265.3 ₄	H 1.95 ₆					B \leftrightarrow X, V?	24738.4 H	(2)
A 0 ⁺	20532.0	135.9 ₁	H 0.53 ₄ ^a	(0.0364)	(0.0002 ₅)		(2.84)	A \leftrightarrow X, R	20495.2 H	(1)* (3)(4)(5)
X 0 ⁺	0	209.5 ₀ ^b	H 0.45	0.04321526	0.000132695 ^c	0.734 ₇	2.60950 ₃	Microwave sp.		(6)
$^{209}\text{Bi}^{35}\text{Cl}$		$\mu = 29.9562508$ $D_0^0 = 3.0_8 \text{ eV}^a$								MAY 1976 A
B	25492.7	403.5 ₀	H 3.76 ₈ ^b					B \leftrightarrow X, V?	25539.5 H	(1)* (2)*
A'	23054.5	217.5	H 2.95	(0.0739) ^c			(2.76 ₀)	A' \leftrightarrow X, R	23008.6 H	(5)(6)* (8)(9)*
A 0 ⁺	21801.8	220.3	H 2.47 ^d	(0.07927) ^c		(3.9)	(2.66 ₄)	A \leftrightarrow X, R	21757.4 H	(1)* (2)* (3)(10)(11)
X 0 ⁺	0	308.4 ^e	H 0.96	(0.0921) ^c		(3.1)	(2.47 ₂)			
$^{209}\text{Bi}^{19}\text{F}$		$\mu = 17.4151900$								MAY 1976 A
C	44222.0	615.0	H 2.50	a				C \leftrightarrow X, V	44274 H	(3)(4)(5)* (14)*
		Two systems ^a (emission only) with $\omega'_e = 611.8$, $\omega''_e = 542.7$ (P, Q heads). $\omega'_e = 614.4$, $\omega''_e = 535.0$						V 36979 H ^Q		(3)(5)*(12)*
B	25986.4	602.0 ^b	H 3.50					V 32179 H		(3)(5)*(13)*
A 0 ⁺	22959.7	381.0	H 3.00 ^c	d				B \leftrightarrow X, ^b	26033 H	(11)
		R shaded emission bands in the region 14350 - 16050 cm^{-1} ; $\omega' \approx 399$, $\omega'' \approx 535$.						A \leftrightarrow X, R	22894.6 H	(1)* (2)(6)* (7)*(8)*(9)*
X 0 ⁺	0	510.7	H 2.05	d						(11)(15)

BiBr: ^a $w_e v_e = -0.103$; convergence limit at 22120 cm^{-1} .
^bFrom the A-X system. Similar constants from B-X.
^c $r_e = +7.68 \times 10^{-8}$.
 (1) Morgan, PR 42, 41 (1936).
 (2) Sur, Majumdar, PNISI 20, 235 (1954).
 (3) Sankaranarayanan, Patel, Narayanan, PIAS A 56, 171 (1962).
 (4) Singh, IJPAP 6, 299 (1968).
 (5) Lal, Mohamed, Khanna, IJPAP 13, 53 (1975).
 (6) Kuijpers, Dymanus, CPL 39, 217 (1976).

BiCl: ^aThermochemical value (7), calculated for a $^3\Sigma$ ground state.
^b $w_e v_e = +0.0016$.
^cRotational analyses by (8)(10)(11); different results in (4)(5)(6). Uncertain.
^d $w_e v_e = -0.02$.
^eFrom the A-X system; similar constants from B-X.
 (1) See ref. (1) of BiBr.
 (2) Ray, IJP 16, 35 (1942).
 (3) Venkateswarlu, Khanna, PIAS A 51, 14 (1960).
 (4) Khanna, JMS 6, 319 (1961).
 (5) Rao, Rao, IJP 39, 65 (1965).
 (6) Babu, Rao, IJPAP 5, 79 (1967).
 (7) Cubicciotti, JPC 71, 3066 (1967).
 (8) Mohanty, Nair, Upadhy, IJPAP 6, 494 (1968).
 (9) Yamdagni, JMS 35, 149 (1970).
 (10) Singh, Upadhy, IJP 45, 121 (1971).
 (11) Rai, Upadhy, Ram, IJP 48, 554 (1974).

BiF: ^aRotational analyses (10)(12)(13)(14).
^bComplex system of V and R shaded bands. The constants above refer to the V shaded heads.
^c $w_e v_e = +0.10$.
^dRotational analyses of several A-X bands in (6)(8) [$B_0' = 0.2097$, $B_0'' = 0.2307$] and (9) [$B_0' = 0.2090$, $B_0'' = 0.2295$].
 (1) Howell, PRS A 155, 141 (1936).
 (2) See ref. (1) of BiBr.
 (3) Rochester, PR 51, 486 (1937).
 (4) Joshi, PPS 78, 610 (1961).
 (5) Rao, Rao, IJP 36, 85 (1962).
 (6) Rao, Rao, CJP 40, 1077 (1962).
 (7) Sankaranarayanan, Narayanan, Patel, PIAS A 59, 378 (1964).
 (8) Rao, Rao, IJP 39, 572 (1965).
 (9) Mohanty, Upadhy, CS 36, 478 (1967).
 (10) Murty, Rao, CS 36, 661 (1967).
 (11) Patel, Narayanan, IJPAP 5, 223 (1967).
 (12) Mohanty, Rai, Upadhy, Singh, JP B 1, 523 (1968).
 (13) Chaudhry, Upadhy, Rai, Mohanty, JP B 1, 1223 (1968).
 (14) Chaudhry, Upadhy, Rai, JP B 2, 628 (1969).
 (15) Murty, Rao, Reddy, Rao, SpL 8, 217 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{209}\text{Bi}^1\text{H}$		$\mu = 1.00298823$ $D_0^0 \leq 2.90 \text{ eV}^a$								MAY 1976
E 0^+	32940.3	[1105.58] Z	30.1	3.5456 ^b	0.0525	[1.401] ^c	2.1772	E \leftarrow X, R	32674.08 Z	(5)(8)
D 1_Σ				[3.88]			[2.08 ₁]	D \rightarrow C, R	20647 Z	(1)(3)
C 1_Σ		[1313.6] Z		4.37	0.11		1.96 ₁			
B 0^+	21263	[1643.07] ^d Z	(47)	5.3078 ^d	0.1861	[2.010] ^e	1.7795	B \rightarrow A, V	16341.72 ^d Z	(1)(3)(4) (6)*
								B \rightarrow X, V	21278.35 ^d Z	(1)* (3)*
A 1 } 3_Σ^-	4917.1	[1669.16] ^f Z	35.4	5.2386 ^{fg}	0.1546	[1.904] ^{fh}	1.7912 ^f			
X 0^+ }	0	[1635.73]	31.6	5.137 ⁱ	0.148	[1.83] ⁱ	1.805			
$^{209}\text{Bi}^2\text{H}$		$\mu = 1.99487609$								MAY 1976
E 0^+	(32929)	j		1.796 ^{kl}	0.0232	m	2.169	E \leftarrow X, R	n	(8)
B 0^+	21263.7	[1185.10] ^d	25.0	2.6687 ^d	0.0644	[0.507] ^o	1.7795	B \rightarrow A, V	16341.10 ^d Z	(4)(6)*
								B \rightarrow X, V	21276.25 ^d Z	(2)(3)
A 1 } 3_Σ^-	4916	[1206.9] ^f	(19)	[2.6084] ^{fg}	0.058	[0.493] ^{fp}	1.790 ^f			
X 0^+ }	0	[1173.32]	16.1	2.592 ⁱ	0.054	[0.506] ⁱ	1.804			

Bi¹H, Bi²H:

- ^aFrom the predissociation in E 0⁺(v=2), assuming dissociation into Bi(²D_{3/2}) + H(²S); see (8).
- ^bLines having v'=1, J' ≥ 16, and all lines with v'=2, are diffuse. The lack of emission from E 0⁺, even from levels which appear sharp in absorption, was attributed (8) to weak predissociation by the Ω=1 component of the repulsive ⁵Σ⁻ state which arises from ground state atoms.
- ^cD₁ = 1.563 x 10⁻⁴.
- ^dConstants from (8).
- ^eD₁ = 2.146 x 10⁻⁴ (8).
- ^fConstants for the f component (8). Ω-type doubling,

$$\left. \begin{array}{l} \text{Bi}^1\text{H: } \Delta v_{ef}(v=0) \approx + 0.0200 \times J(J+1) - \dots \\ \text{Bi}^2\text{H: } \Delta v_{ef}(v=0) \approx + 0.0049 \times J(J+1) - \dots \end{array} \right\} (6)(8).$$
- ^gMagnetic hyperfine structure (4)(6)(7).
- ^hD₁ = 1.915 x 10⁻⁴; also higher order constants (8).
- ⁱEffective constants; see also (8).
- ^jΔG(3/2) = 768.75. Using isotope relations: ω_e ≈ 829.3,
 ω_ex_e ≈ 15.1.
- ^kExtrapolated from B₁ = 1.7607 and B₂.
- ^lSlight broadening of lines having v'=2, J' ≥ 18. v'=3 not observed.
- ^mD₁ = 0.378 x 10⁻⁴, D₂ = 0.423 x 10⁻⁴.
- ⁿv₀(1-0) = 33540.58.
- ^oD₁ = 0.528 x 10⁻⁴ (8).
- ^pD₁ = 0.489 x 10⁻⁴; higher order constants in (8).

- (1) Heimer, ZP 95, 328 (1935).
- (2) Heimer, ZP 103, 621 (1936).
- (3) Heimer, Dissertation (Stockholm, 1937).
- (4) Hulthén, Neuhaus, PR 102, 1415 (1956).
- (5) Khan, Khan, PPS 88, 211 (1966).
- (6) Neuhaus, ZN 21 a, 2113 (1966).
- (7) T. M. Dunn, in "Molecular Spectroscopy: Modern Research", edited by K. N. Rao and C. W. Mathews; p. 231. Academic Press (1972).
- (8) Lindgren, Nilsson, JMS 55, 407 (1975).

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻⁸ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
								Design.	ν ₀₀		
²⁰⁹Bi¹²⁷I											
		μ = 78.957256 ₀								MAY 1976	
C	40707.1	230.9	H	4.75				C←X,	40739.5	H (3)	
		Unclassified absorption bands in the region 24100 - 25000 cm ⁻¹ .								(5)	
B	23389.1	198.0 ₉	H	1.44 ₄ ^a				(B→a), ^b R	17213.5	H (2)(4)*	
								B↔X,	R 23405.9	H (1)(2)(6)*	
A'	20318.7	126.8	H	0.90				A'←X,	R 20300.0	H (5)	
A	20006.0	145.0	H	2.50				A←X,	R 19996.0	H (5)	
a	(6190)	170.8	H	0.3							
X 0 ⁺	0	163.8 ₈	H	0.28 ₀ ^c	0.027222814	0.000069790 ₆ ^d	0.29959 ^e	2.80050 ₁	Microwave sp.	(7)	
²⁰⁹Bi¹⁶⁰O											
		μ = 14.8577355 ₇ D ₀ ⁰ = 3.47 eV ^a								MAY 1976	
F	(40941)	[748]	H	Fragments only.				F←X ₁ ,	40970	H (2)*	
E (² Σ?)	38550	769.3	H	6.2				E←X ₁ ,	38588	H (2)*	
D (² Π) _{1/2}	(32805)	(343)			[0.228 ₄] ^{bc}	[45]	[2.229]	D←X ₁ ,	R 32631.35	Z (6)*	
C (² Δ) _{3/2}	(30700)	(465)			[0.2548] ^{de}	[30.6]	[2.1102]	C←X ₁ , ^f R	30587.16 ^d	Z (6)*	
B ⁴ Σ _{1/2} ⁻	28738.2	483		5	0.260 ^g	0.0029	^h	2.09	B↔X ₁ , ^f R	28633.35	Z (2)(5)* (6)*
A ² Π _{1/2}	14187.0	508.8	Z	2.78	0.24715 ⁱ	0.00167	23.3	2.1426	A↔X ₁ , ^f R	14095.6	Z (1)(3)(4)* (6)*
X ₂ ² Π _{3/2}	(8000)										
X ₁ ² Π _{1/2}	0	692.4	Z	4.34	0.3034 ^{jc}	0.0022	[22.1]	1.934			

BiI: ^aAlso higher order constants.

^bIt is not certain that the upper state of this system ($w'_e = 200.6$, $w'_e x'_e = 1.4$) is identical with the B state observed in absorption and emission.

^c $w_e y_e = -0.005$.

^d $+1.72_1 \times 10^{-8} (v+\frac{1}{2})^2 - 9.9 \times 10^{-11} (v+\frac{1}{2})^3$.

^e $\beta_e = +0.00035_4 \times 10^{-8}$.

(1) See ref. (1) of BiBr.

(2) Rao, IJP 23, 379 (1949).

(3) M. M. Joshi, Thesis (Allahabad University, 1958).
Quoted in (5).

(4) Singh, IJPAP 6, 445 (1968).

(5) Yamdagni, SA A 26, 1071 (1970).

(6) Singh, Asthana, Singh, SpL 8, 101 (1975).

(7) Kuijpers, Törring, Dymanus, CP 12, 309 (1976).

BiO: ^aThermochemical value (mass-spectrom.) (9).

^bBoth high and low rotational levels are predissociated; the e and f levels were only observed for $43.5 \leq J \leq 71.5$ and $57.5 \leq J \leq 81.5$, resp.. In this region, the Ω -type doubling [recalc. from (6)] is well represented by $\Delta v_{fe} = (+)[0.306 - 11.09 \times 10^{-6} (J+\frac{1}{2})^2] (J+\frac{1}{2})$.

^cUnresolved magnetic hyperfine structure; see (6)(7).

^dVibrational numbering uncertain. The single band reported by (6) agrees in position with the 1-0 band of a weak system observed by (2) at about 1480 cm^{-1} above the B-X bands.

^eVery small Ω -type doubling.

^fThe lines have half-widths of $\sim 0.25 \text{ cm}^{-1}$ (independent of J), owing to the unresolved magnetic hyperfine splitting of the ground state levels.

BiO (continued):

^gLarge Ω -type doubling, $\Delta v_{fe}(v, J) = p_v(J+\frac{1}{2}) - \dots$ where $p_v \approx +4B_v$ (6). The sign of the splitting can not be determined from the spectrum but is chosen here to give agreement with theoretical predictions [see (8)] for a $4\Sigma^-$ state. This requires the parities of most rotational levels in figure 4 of (6) to be reversed and leads to negative values of Δv_{fe} in the ground state of BiO, contrary to results for other group V oxides.

^h D_v increases from $D_2 = 32.3 \times 10^{-8}$ to $D_5 = 80.3 \times 10^{-8}$ [see (6)].

ⁱ $\Delta v_{fe}(v=2, \dots, 9) \approx (+)0.025(J+\frac{1}{2}) - \dots$; for more details see (6).

^j $\Delta v_{fe}(v=0) = (-)0.187(J+\frac{1}{2})$.

(1) Sen Gupta, IJP 18, 182 (1944).

(2) Bridge, Howell, PPS A 67, 44 (1954).

(3) Scari, APH 6, 73 (1956).

(4) Gissane, Barrow, PPS 85, 1048 (1965); 86, 682 (1965)(Corrigendum).

(5) Babu, Rao, CJP 44, 705 (1966).

(6) Barrow, Gissane, Richards, PRS A 300, 469 (1967).

(7) Atkins, PRS A 300, 487 (1967).

(8) Kopp, Hougén, CJP 45, 2581 (1967).

(9) Uy, Drowart, TFS 65, 3221 (1969).

(10) Rao, Lakshman, CS 40, 316 (1971).

(11) Asthana, Kushawaha, Nair, APP A 42, 739 (1972).

(12) Singh, Shukla, JQSRT 12, 1249 (1972).

(13) Singh, JQSRT 12, 1343 (1972).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References		
								Design.	ν_{00}			
$^{209}\text{Bi}^{32}\text{S}$		$\mu = 27.7296867$ $D_0^0 = 3.17 \text{ eV}^a$ One of two systems of ultra-violet bands attributed (1) to BiS is, in fact, the B-X system of S_2 [see (4)]. The other, consisting of V(?) shaded bands in the region $43200 - 46900 \text{ cm}^{-1}$, appears to include bands which the same author (2) also assigned to SbS. In the latter case the bands were described as red-degraded.								MAY 1976		
A	$2\Pi_{1/2}$	≤ 13343.9	$\geq 303.74^b$	H	1.159	$\geq 0.09258^{bc}$	0.000416	3.5 ₅	≤ 2.563	$A \leftarrow X,^d$ R $\leq 13291.5^b$	H	(4)
X	$2\Pi_{1/2}$	0	408.71	H	1.46	$[0.112764]^e$	(0.000486)	[3.34]	2.3194			
$^{209}\text{Bi}^{(80)}\text{Se}$		$(\mu = 57.809502_2)$ $D_0^0 = 2.80 \text{ eV}^a$										MAY 1976
D	44425	316.0	H	2.0						$D \leftarrow X,$ V 44450	H	(1)
C	35618	304.0	H	2.0						$C \leftarrow X,$ V 35637	H	(1)
B	20411	169.4	H	0.8						$B \leftarrow X,$ R 20363	H	(5)
A	$\frac{1}{2}$	≤ 13235.7	$\geq 190.9^b$	H	0.595^b					$A \leftarrow X,^c$ R ≤ 13198.3	H	(3)
X	$\frac{1}{2}$	0	$[264.8]^b$	H	0.4							
$^{209}\text{Bi}^{(130)}\text{Te}$		$(\mu = 80.108962_1)$ $D_0^0 = 2.4_0 \text{ eV}^a$										MAY 1976
		Bands in the region $43900 - 45300 \text{ cm}^{-1}$.										
E										$E \leftarrow X,$ V		(1)
D	43116	263.0	H	0.96						$D \leftarrow X,$ V 43143	H	(1)
C	(42870)	(164.4)	H	(0.4)						$C \leftarrow X,$ (V) (42848)	H	(1)
B		Bands in the region $40700 - 42000 \text{ cm}^{-1}$.										
A		Bands in the region $34000 - 35500 \text{ cm}^{-1}$.										
X	0	208.5	H	0.52						$A \leftarrow X,$ V		(1)

BiS: ^aThermochemical value (mass-spectrom.)(5); (3).

^bVibrational numbering uncertain.

^c $|\Delta v_{\text{Fe}}| \approx 0.006(J+\frac{1}{2}) [v=7,8]$.

^dLine widths of 0.45 cm^{-1} result from unresolved nuclear magnetic hyperfine structure.

^eLarge Ω -type doubling, $|\Delta v_{\text{Fe}}(v=0)| = 0.1135(J+\frac{1}{2})$.

(1) Sur, IJP 25, 65 (1951).

(2) Sur, PNASI A 20, 251 (1951).

(3) Cubicciotti, JPC 67, 118 (1963).

(4) Barrow, Stobart, Vaughan, PPS 90, 555 (1967).

(5) See ref. (9) of BiO.

(6) Singh, Pandey, IJPAP 7, 580 (1969).

(7) Asthana, APP A 42, 739 (1972).

BiSe: ^aThermochemical value (mass-spectrom.)(2)(4).

^bConstants for Bi⁸⁰Se.

^cBroad lines on account of unresolved nuclear magnetic hyperfine structure.

(1) Sharma, PPS A 67, 935 (1954).

(2) Porter, Spencer, JCP 32, 943 (1960).

(3) See ref. (4) of BiS.

(4) See ref. (9) of BiO.

(5) Yamdagni, IJPAP 8, 51 (1970).

BiTe: ^aThermochemical value (mass-spectrom.)(2)(4); (3).

(1) See ref. (1) of BiSe.

(2) See ref. (2) of BiSe.

(3) Boncheva-Mladenova, Pashinkin, Novoselova, IANNM 4, 291 (1968).

(4) See ref. (9) of BiO.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{11}\text{B}^{14}\text{N}$		$\mu = 6.1635127_6$ Incompletely analyzed singlet transitions (in emission).						R 34499 H R 32817 H V 30963 H A \leftrightarrow X, R 27775.8 H	JUN 1976 (1) (1)* (2)(3) (5)	
A $^3\Pi$	27875.0	1317.5	H 14.9	1.555	0.010	(8.7)	1.326			
X $^3\Pi^a$	0	1514.6	H 12.3	1.666	0.025	(8.1)	1.281			
$^{11}\text{B}^{16}\text{O}$		$\mu = 6.5209400_9$ $D_0^0 = 8.28 \text{ eV}^a$								JUN 1976
C $^2\Pi_{(r)}$	55346.1 ^b	1315.3	H 11.1	1.483	0.018	8	1.320	C \rightarrow X, γ -bands R	55061.5 ^c	(7)* (10) (11)*
B $^2\Sigma^+$	43174.05	1281.69	Z 10.66	1.5171 ^{de}	0.0210	8.5	1.3054	B \rightarrow A, ^f V	19225.9 19351.0	(1)
A $^2\Pi_i$	23958.76 ^h 23833.7	1260.70	Z 11.157 ⁱ	[1.4018] ^{je}	0.0196	[7.63]	1.3533	B \rightarrow X, β -bands R	42872.34 Z	(1)* (3)* (6)(8)*
X $^2\Sigma^+$	0	1885.69	Z 11.81	1.7820 ^{me}	0.0166	6.32 ⁿ	1.2045	A \leftrightarrow X, α -bands R	23646.43 ^d Z 23521.3 ^l Z	(1)* (2)* (4)* (5)* (14)(18)
$^{11}\text{B}^{16}\text{O}^+$										JUN 1976
b $^1\Sigma$	(27941)	(1952)		[1.8202]		[6.33]	[1.1917]	b \rightarrow a, V	28023.99 Z	(16a)
a $^1\Sigma$	(0)	(1787)		[1.7799]		[7.06]	[1.2052]			
$(^{11})\text{B}^{16}\text{O}^-$		I.P. = 3.1 ₂ eV ^p								JUN 1976 A
$(^{11})\text{B}^{31}\text{P}$		$(\mu = 8.1223128_4)$ $D_0^0 = 3.5_6 \text{ eV}^a$								JUN 1976

BN: ^aThe observation of A←X in absorption in rare gas matrices (5) supports theoretical predictions (4)(6) of a ³Π ground state.

- (1) Douglas, Herzberg, CJR A 18, 179 (1940).
- (2) Nicholls, Fraser, Jarman, CF 3, 13 (1959).
- (3) Thrush, Nature 186, 1044 (1960).
- (4) Verhaegen, Richards, Moser, JCP 46, 160 (1967).
- (5) Mosher, Frosch, JCP 52, 5781 (1970).
- (6) Melrose, Russell, JCP 55, 470 (1971); 57, 2586 (1972).

BO, BO⁺, BO⁻:

^aThermochemical value (mass-spectrom.)(17)(19); in good agreement with 8.3 eV by flame photometry (15).

^bA = (+)46.4.

^cR₂ head at 55084.2 cm⁻¹.

^dSpin splitting constant γ ≈ + 0.025 (8)(18).

^ePotential curves (16).

^fFranck-Condon factors (9).

^gFranck-Condon factors (9)(13)(21); measured relative intensities (13).

^hA₀ = - 122.26 (slight J dependence)(18); A₁ = - 122.36 (5).

ⁱw_ey_e = + 0.049.

^jΛ-type doubling in ²Π_{1/2}, Δv_{fe} ≈ + 0.025(J+½) - ... (5)(18); for ²Π_{3/2} see (5).

^kFranck-Condon factors (9)(12)(13)(21); measured relative (13) and estimated absolute (22) intensities.

^l{J'=0} relative to N''=0.

^mFrom (8); slightly different constants in (5). Spin splitting constant γ(v=2) = + 0.0065 (18).

ⁿβ_e = + 0.02 x 10⁻⁶.

^oIn rare gas matrices at 4 K (20).

^pFrom the heat of formation for BO⁻ (21a).

BO, BO⁺, BO⁻ (continued):

- (1) Mulliken, PR 25, 259 (1925).
- (2) Jenkins, PNASU 13, 496 (1927).
- (3) Elliot, PKNAW 32, 644 (1930); 38, 736 (1935).
- (4) Scheib, ZP 60, 74 (1930).
- (5) Jenkins, McKellar, PR 42, 464 (1932).
- (6) Funke, Simons, PKNAW 38, 142 (1935).
- (7) Chrétien, HPA 23, 259 (1950).
- (8) Lagerqvist, Nilsson, Wigartz, AF 13, 379 (1958).
- (9) See ref. (2) of BN.
- (10) Kuzyakov, Tatevskii, Tunitskii, OS(Engl. Transl.) 2, 84 (1960).
- (11) Mal'tsev, Kataev, Tatevskii, OS(Engl. Transl.) 2, 376 (1960).
- (12) Nicholls, Fraser, Jarman, McEachran, ApJ 131, 399 (1960).
- (13) Robinson, Nicholls, PPS 75, 817 (1960).
- (14) See ref. (3) of BN.
- (15) De Galan, Physica 31, 1286 (1965).
- (16) Singh, Rai, JQSRT 5, 723 (1965).
- (16a) Kataev, Mal'tsev, VMUK 22 (2), 23 (1967).
- (17) Coppens, Smoes, Drowart, TFS 64, 630 (1968).
- (18) Dunn, Hanson, CJP 47, 1657 (1969).
- (19) Uy, Drowart, HTS 2, 293 (1970).
- (20) Knight, Easley, Weltner, JCP 54, 1610 (1971).
- (21) Liszt, Smith, JQSRT 11, 1043 (1971).
- (21a) Srivastava, Uy, Farber, TFS 67, 2941 (1971).
- (22) Kuz'menko, Kuznetsova, Kuzyakov, Chuev, JAS 20, 373 (1974).

BP: ^aThermochemical value (mass-spectrom.)(1).

- (1) Gingerich, JCP 56, 4239 (1972).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁸ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
								Design.	v ₀₀		
⁷⁹ Br ₂		μ = 39.459166 ₀ D ₀ ⁰ = 1.9707 ₀ eV ^a I.P. = 10.52 eV ^b Fragments of additional Rydberg series converging to A ² Π _u of Br ₂ ⁺ . Rydberg series converging to X ₂ ² Π _{g,1/2} of Br ₂ ⁺ : v = 88306 ^c - $\left\{ \begin{array}{l} R/(n-2.416)^2 \\ R/(n-2.446)^2 \\ R/(n-2.591)^2 \\ R/(n-2.629)^2 \end{array} \right\} n = 5, 6, 7.$ Rydberg series converging to X ₁ ² Π _{g,3/2} of Br ₂ ⁺ : v = 85165 ^d - $\left\{ \begin{array}{l} R/(n-1.843)^2, n = 5, \dots, 12. \\ R/(n-1.938)^2, n = 5, \dots, 18. \\ R/(n-2.225)^2 \\ R/(n-2.422)^2 \\ R/(n-2.593)^2 \end{array} \right\} n = 5, \dots, 20.$							SEP 1976 A (18)* (18)* (18)*		
	N	76537	230 ^e	H				N ← X,	R 76491	H	(18)*
	M	74060	241 ^e	H (0.3)				M ← X,	R 74019	H	(18)*
	L	72727	218 ^e	H 3				L ← X,	R 72674	H	(18)*
		Several groups of diffuse emission bands in the region 23600 - 50000 cm ⁻¹ have been assigned (5) to transitions from four states at 47000, 55534, 61444, 66500 cm ⁻¹ to various repulsive states arising from Br(² P _{3/2,1/2}) + Br(² P _{3/2,1/2}).								(5)	
(K)		Extensive system of absorption bands in the region 59000 - 67000 cm ⁻¹ ; no analysis. This system may include transitions to the upper states of: a) three emission systems, M → X of (9), with w' ≈ $\begin{array}{l} 293^e \\ 426^e \\ 281^e \end{array}$; b) a long resonance series (63817 - 53779 cm ⁻¹).						(K) ← X,		(18)	
								R 62266	H	(9)	
								V 60879	H		
								R 59855	H	(12)	
H	(56820)	108.0 ^{ef}	1.5					H → B,	(40890) ^f		(10)
G	56337	(255) ^e	H					G → X, ^g	R 56303	H	(9)
F	52191	(120) ^e	H					F → X, ^h	R 52090	H	(9)
E	51634.0	150.9 ^e	0.49 ₅ ⁱ					E ↔ B ^j ,	35724.0 ^e		(7)(11)(28)

Br₂: ^aFrom (32); corresponding values for ^{79,81}Br₂ and ⁸¹Br₂ are 1.9708₂ and 1.9709₅ eV (short extrapol. of B O_u⁺).
^bFrom photoionization (21); supported by measurements at different temperatures. In good agreement with 10.51 eV obtained by photoelectron spectroscopy (15)(23)(26). A slightly higher value, 10.56 eV, was derived (18) from the Rydberg series in the VUV. It is probable that this value refers to v'=1.
^cThe interval of 3141 cm⁻¹ between X₁ ²Π_{3/2} and X₂ ²Π_{1/2} of Br₂⁺ derived from the Rydberg series does not agree with the value 2820 cm⁻¹ from the photoelectron spectrum (23). The discrepancy may be accounted for by assuming that instead of v'=0 as suggested in (18) the ²Π_{1/2} series listed here have v'=2 while the ²Π_{3/2} series have v'=1 (see ^d).
^dAccording to the photoionization and photoelectron value of the ionization potential (see ^b) the five ²Π_{3/2} Rydberg series in the table refer to v'=1. Vibrational structure; see (18).
^eNormal isotopic mixture.

^fThe vibrational analysis is doubtful since only v''=21-32 were observed. v₀₀ (extrapolated) and T_e are different from (10) to allow for the new data on the B state (32).
^gSystem J-X of (9), not observed in absorption.
^hSystem H-X of (9), not observed in absorption.
ⁱw_ez_e = + 0.00006₅; vibrational constants from the reanalysis (28) of the emission data of (7) and the absorption data of (11). See ^j.
^jIt is not entirely certain that the lower state is B ³Π_{u,0}⁺ and not A ³Π_{u,1}.
(continued p.106)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions Design. v_{00}	References
$^{79}\text{Br}_2$ (continued)									
D	48499	162.0 ^e	0.29					D \rightarrow B, 32595	(8)
C $^1\Pi_u$ $^1\Pi_u$ (24000)		Several absorption continua beyond 19580 cm^{-1} corresponding to a number of electronic transitions including that to C $^1\Pi_u$ with maximum at 24000 cm^{-1} .						C ^k \leftarrow X, (24000)	(1)(2)(3)(4) (6)(30a)
B $\left\{ \begin{array}{l} 0_u^+ \\ 3\Pi_u \end{array} \right.$	15902.47	167.607	Z	1.6361 ^l	0.059589 ^{mno}	0.00048910 ^p	3.013 ^q	2.6775 ₇ B ^{kr} \leftrightarrow X, ^o R 15823.47 Z	(16)* (24)* (20)(32)(35)
A $\left\{ \begin{array}{l} 1_u \\ 1_u \end{array} \right.$	13905	153 ^e	H	2.7 ^s	0.0588 ^{tu} (0.0008)		2.69 ₅	A ^{kr} \leftrightarrow X, ^u R 13818 ^v	(13)(14)* (29)
X $^1\Sigma_g^+$	0	325.321	Z	1.0774 ^w	0.082107 ^x	0.0003187 ^y	2.092 ^q	2.2810 ₅ Raman sp. ^z	

Br₂ (continued):

^kAlso observed in magnetic circular dichroism (38) and photofragment (40) spectra. The latter authors confirm Mulliken's (3) prediction that C $^1\Pi_u$ dissociates into $^2P_{3/2} + ^2P_{3/2}$ and observe evidence for several excited g states by two-photon photofragment studies near 28000 and 38000 cm^{-1} .

^l $\omega_e y_e = -0.009369$ (for $v \leq 8$). Vibrational levels observed to $v=55$, dissociation limit ($^2P_{3/2} + ^2P_{3/2}$) at 19579.76 cm^{-1} above X $^1\Sigma_g^+(v=0, J=0)$. See ^o. Absorption in the B 0_u^+ continuum (43).

^mHfs observed in $v=12$ ($^{81}\text{Br}_2$) and $v=17$ ($^{79}\text{Br}_2$); see (33).

ⁿPredissociation was observed (41)(39) for $v=42, J=33$ by the laser-molecular beam technique. B \rightarrow X emitted in the recombination of Br($^2P_{3/2}$) atoms shows strong enhancement of bands with $5 < v' < 10$ presumably on account of inverse predissociation (27). See also ^r.

^oRKR potential function and Franck-Condon factors (25)(32). For the behaviour of the potential function near the dissociation limit^t see (30)(31)(34).

^p $r_e = -6.637 \times 10^{-6}$ (valid for $v \leq 8$).

^q D_v and higher order constants in (32).

^rEstimated radiative lifetimes for A and B range from 1000 to 2000 and 12 to 70 μs , respectively (29)(30a)(43). For the B state (22) find total lifetimes of the order of 1 μs ; minima ($\sim 0.2 \mu\text{s}$) occur for $v=1$ and 14 probably on account of predissociation. For lifetimes near the dissociation limit^t of B see (42).

^sConvergence limit for $^{79}\text{Br}_2$ at 15894.6 cm^{-1} above X $^1\Sigma_g^+(v=0, J=0)$, corresponding to $^2P_{3/2} + ^2P_{3/2}$. A weak continuous spectrum joins onto the limit and overlaps the main absorption system B \leftarrow X; see (17).

^tExtrapolated from $v=7$; constants for $v=0\dots 6$ have not been

Br₂ (continued):

determined. B_v, D_v, H_v, and Λ-type doubling constants for v=7...24 in (29).

^uRKR potential function and Franck-Condon factors (29).

^vBased on AG'(v=0-7) from low-resolution emission spectra (14) of normal Br₂ and the origin of the 7-0 ⁷⁹Br₂ band at 14739.14 cm⁻¹ derived from (29) and (32).

^wy_e = -0.002298.

^xRKR potential curve (25)(32). Hfs observed (33) in v=4 (⁸¹Br₂) and v=7 (⁷⁹Br₂).

^yy_e = -1.04₅ x 10⁻⁶.

^zResonance Raman spectra in the gas (19)(37), in solid argon (35); pure rotational Raman spectrum (36).

(1) Cordes, Sponer, ZP 63, 334 (1930).

(2) Aickin, Bayliss, TFS 34, 1371 (1938).

(3) Mulliken, PR 57, 500 (1940).

(4) Rees, PPS 59, 1008 (1947).

(5) Venkateswarlu, PIAS A 25, 138 (1947).

(6) Bayliss, Sullivan, JCP 22, 1615 (1954).

(7) Venkateswarlu, Verma, PIAS A 46, 251 (1957).

(8) Venkateswarlu, Verma, PIAS A 46, 416 (1957).

(9) Haranath, Rao, JMS 2, 428 (1958).

(10) Verma, PIAS A 47, 196 (1958).

(11) Briggs, Norrish, PRS A 276, 51 (1963).

(12) Rao, Venkateswarlu, JMS 13, 288 (1964).

(13) Horsley, JMS 22, 469 (1967).

(14) Clyne, Coxon, JMS 23, 258 (1967).

(15) Frost, McDowell, Vroom, JCP 46, 4255 (1967).

(16) Horsley, Barrow, TFS 63, 32 (1967).

(17) Sulzmann, Bien, Penner, JQSRT 7, 969 (1967).

(18) Venkateswarlu, CJP 47, 2525 (1969).

(19) Holzer, Murphy, Bernstein, JCP 52, 399 (1970).

(20) Holzer, Murphy, Bernstein, JCP 52, 469 (1970).

(21) Dibeler, Walker, McCulloh, JCP 53, 4715 (1970).

(22) Capelle, Sakurai, Broida, JCP 54, 1728 (1971).

(23) Cornford, Frost, McDowell, Ragle, Stenhouse, JCP 54, 2651 (1971).

(24) Coxon, JMS 37, 39 (1971).

(25) Coxon, JQSRT 11, 443 (1971); 12, 639 (1972).

(26) Potts, Price, TFS 67, 1242 (1971).

(27) Clyne, Coxon, Woon-Fat, TFS 67, 3155 (1971).

(28) Wieland, Tellinghuisen, Nobs, JMS 41, 69 (1972).

(29) Coxon, JMS 41, 548, 566 (1972).

(30) Goscinski, MP 24, 655 (1972).

(30a) Coxon, in "Molecular Spectroscopy", Vol. 1, p. 177. The Chemical Society (1973).

(31) Yee, Stone, MP 26, 1169 (1973).

(32) Barrow, Clark, Coxon, Yee, JMS 51, 428 (1974).

(33) Eng, LaTourrette, JMS 52, 269 (1974).

(34) Le Roy, CJP 52, 246 (1974).

(35) Ault, Howard, Andrews, JMS 55, 217 (1975).

(36) Baierl, Hochenbleicher, Kiefer, AS 29, 356 (1975).

(37) Baierl, Kiefer, JCP 62, 306 (1975).

(38) Brith, Rowe, Schnepf, Stephens, CP 2, 57 (1975).

(39) Lum, Hozack, JMS 58, 325 (1975).

(40) Oldman, Sander, Wilson, JCP 63, 4252 (1975).

(41) Lum, McAfee, JCP 63, 5029 (1975).

(42) McAfee, Hozack, JCP 64, 2491 (1976).

(43) Bondybey, Bearder, Fletcher, JCP 64, 5243 (1976).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(79,81) \text{Br}_2^+$										
$(\mu = 39.952275) \quad D_0^0 = 3.26 \text{ eV}^a$										JUN 1976
Highly excited X-ray states obtained in heavy ion collisions ($\text{Br}^+ + \text{Br}$), discussed in (4).										
Third state observed in the photoelectron spectrum (2)(3).										
$(^2\Sigma_g^+)$ (30700)										
$A_2(^2\Pi_u)$ $\left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{3}{2} \end{smallmatrix} \right.$ 21602 ^b		152.0	0.35					$A_2 \rightarrow X_2$,	18670	(1)*
$A_1(^2\Pi_u)$ $\left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{3}{2} \end{smallmatrix} \right.$ 19290 ^b		190.0	1.0					$A_1 \rightarrow X_1$,	19197	(1)*
$X_2(^2\Pi_g)$ $\left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{3}{2} \end{smallmatrix} \right.$ 2820 ^c		376.0	1.25							
$X_1(^2\Sigma_g^+)$ $\left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{3}{2} \end{smallmatrix} \right.$ 0										
$(79,81) \text{Br}_2^-$										
$(\mu = 39.952549) \quad D_0^0 = 1.15 \text{ eV}^a \quad \text{I.P.} = 2.55 \text{ eV}^b$										JUN 1976
$(^2\Pi_g)$ $\left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{3}{2} \end{smallmatrix} \right.$ [77500]		363 ^c								(4)
$X(^2\Sigma_u^+)$ [0]										
$^{79}\text{Br}^{35}\text{Cl}$										
$\mu = 24.2317306 \quad D_0^0 = 2.23_3 \text{ eV}^a \quad \text{I.P.} = 11.1 \text{ eV}^b$										JUN 1976 A
Additional absorption bands above 65000 cm^{-1} ; no analysis.										(1)* (8)*
Six continuous emission bands between 27800 and 39200 cm^{-1} .										(5)
D 61570		[504] ^c H						$D \leftrightarrow X$, V	61600 H	(1)* (5)
C 59325		519 ^c H 2.9						$C \leftrightarrow X$, V	59362 H	(1)* (5)
B $^3\Pi_0^+$ 16879.91 ^d		222.68 ^d 2.884 ^d		0.107704 ^{ef}		(1.0 ₁)	2.5415	$B \leftrightarrow X$, 3R	16735.9 ^h	(7)* (12) (13)(14)
A $^3\Pi_1$		Several bands of this system observed but not analysed.						$A \leftarrow X$, R		(12)
X $^1\Sigma^+$ 0		444.27 ₆ Z 1.843 ⁱ		0.152469 ₅ ^f 0.000769 ₇ ^j		0.7183 ^k	2.13606 ₅	Infrared sp. ^l		(3)(4)(7)
								Raman sp. ^m		(9)
								Microwave sp. ⁿ		(2)

- Br_2^+ : ^a $D_0^0(\text{Br}_2) + \text{I.P.}(\text{Br}) [= 11.8139 \text{ eV (1a)}] - \text{I.P.}(\text{Br}_2)$.
^bThe energies of the two $^2\Pi_u$ components fit moderately well with two partially resolved peaks at ~ 12.8 and 13.1 eV in the photoelectron spectrum (2)(3). The rather large difference between the w_e values in the two components raises some doubt in the correctness of the analysis.
^cFrom the photoelectron spectrum (2)(3).
 (1) Haranath, Rao, IJP 29, 205 (1955).
 (1a)Tech, JRNBS A 67, 505 (1963).
 (2) Cornford, Frost, McDowell, Ragle, Stenhouse, JCP 54, 2651 (1971).
 (3) Potts, Price, TFS 67, 1242 (1971).
 (4) Soff, Müller, LNC 2, 557 (1974).
- Br_2^- : ^a $D_0^0(\text{Br}_2) + \text{I.P.}(\text{Br}_2^-) - \text{I.P.}(\text{Br}^-)$.
^bFrom endoergic charge transfer (2)(3)(3a)(5). Dissociative electron attachment gives the slightly higher value of 2.87 eV (1).
^cFrom two progressions of resonances in the scattering of electrons by Br_2 indicating the existence of a pre-ionized doubly excited state of Br_2^- with the $X^2\Pi_g$ state of Br_2^+ as "grandparent" (4).
 (1) DeCorpo, Franklin, JCP 54, 1885 (1971).
 (2) Chupka, Berkowitz, Gutman, JCP 55, 2724 (1971).
 (3) Baede, Physica 59, 541 (1972).
 (3a)Hughes, Lifshitz, Tiernan, JCP 59, 3162 (1973).
 (4) Spence, PR A 10, 1045 (1974).
 (5) Tang, Leffert, Rothe, Reck, JCP 62, 132 (1975).
- BrCl : ^aFrom the heats of formation of BrCl and Br_2 (10) and the dissociation energies of Br_2 and Cl_2 .
^bElectron impact appearance potential (6).
^cNormal isotopic mixture.
^dDeperturbed constants (12) allowing for the perturbation

BrCl (continued):

- by the intersecting 0^+ state arising from normal atoms (interaction matrix element $\approx 360 \text{ cm}^{-1}$); $w_e y_e = -0.0673$.
 The observed vibrational levels (12) are pushed down from their calculated positions by shifts ranging from 42 (for $v=2$) to $135 \text{ (for } v=8) \text{ cm}^{-1}$.
^eDeperturbed value (12); α_e not given. Experimental B_v , D_v , ^fRKR potential curve (12). H_v values for $2 \leq v \leq 8$ in (12).
^gFranck-Condon factors (12).
^hExtrapolated from the lowest observed level ($v'=2$); see (12). (7) give 16695 cm^{-1} based on low-dispersion spectra.
ⁱ $w_e y_e = -0.0040$.
^j $y_e = -26 \times 10^{-7}$.
^k $\beta_e = +0.0035 \times 10^{-7}$; $H_e = -1.53 \times 10^{-14}$.
^lIntegrated abs. coefficients, dipole moment derivative (4).
^mSee also (11) [liquid BrCl] and (14) [BrCl in rare gas matrices].
ⁿ $\mu_{el} \approx 0.57 \text{ D}$ and values of $\text{eqq}(^{35,37}\text{Cl}, ^{79,81}\text{Br})$.
 (1) Cordes, Sponer, ZP 79, 170 (1932).
 (2) Smith, Tidwell, Williams, PR 79, 1007 (1950).
 (3) Mattraw, Pachucki, Hawkins, JCP 22, 1117 (1954).
 (4) Brooks, Crawford, JCP 23, 363 (1955).
 (5) Haranath, Rao, IJP 31, 368 (1957).
 (6) Irsa, Friedman, JINC 6, 77 (1958).
 (7) Clyne, Coxon, PRS A 298, 424 (1967).
 (8) Donovan, Husain, TFS 64, 2325 (1968).
 (9) Holzer, Murphy, Bernstein, JCP 52, 399 (1970).
 (10) JANAF (1971).
 (11) Wallart, CJS 17, 128 (1972).
 (12) Coxon, JMS 50, 142 (1974).
 (13) Hadley, Bina, Brabson, JPC 78, 1833 (1974).
 (14) Wight, Ault, Andrews, JMS 56, 239 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{79}\text{Br}^{19}\text{F}$		$\mu = 15.3122179$ $D_0^0 = 2.54_8 \text{ eV}^a$ I.P. = 11.78 eV^b Fragments of three emission systems between 57000 and 64000 cm^{-1} .								JUN 1976 A
B $^3\Pi_0^+$	18272.0	372.2	H 3.49 ^c					B \leftrightarrow X, R	18122.8 H	(4) (2)(3)(8)*
A $^3\Pi_1$	(17385)	(378) ^d	H (16)					A \leftarrow X, R	(17235) ^d	(3)
X $^1\Sigma^+$	0	670.75	H 4.054	0.35584_3^e	0.00261_2	(0.401)	1.75894	Microwave sp. ^f		(1)
$(^{79})\text{Br}^{19}\text{F}^+$		$D_0^0 = 2.61 \text{ eV}^g$								JUN 1976
X ₂ $^2\Pi_{1/2}$	2600 ^h	750 ^h								
X ₁ $^2\Pi_{3/2}$	0									
$^{79}\text{Br}^{16}\text{O}$		$\mu = 13.2994292_5$ $D_0^0 = 2.39_7 \text{ eV}^a$ d								JUN 1976
A ($^2\Pi_{3/2}$)	27871	485.9 ^b	H 5.40 ^c					A \leftrightarrow X ₁ , R	27725 ^b H	(1)(2)*
X ₂ $^2\Pi_{1/2}$	(900) ^e									
X ₁ $^2\Pi_{3/2}$	0	778.7 ^b	H 6.8 ₂	0.429598^f	0.003639	(0.523)	1.717_2^g	Microwave sp. ^h EPR sp.		(4)(7) (5)(8)
$^{11}\text{B}^{32}\text{S}$		$\mu = 8.1893677_4$ $D_0^0 = 6.01 \text{ eV}^a$								JUN 1976 A
G $^2\Sigma$				$[0.6148]^b$		[0.89]	$[1.829_8]$	G \rightarrow F, V	19506.94 Z 19829.62 Z	(3)*
F $^2\Pi_i$	c			$[0.5782]^d$ $[0.5760]$		[0.81]	$[1.888_6]$			
D $^2\Delta_i$	(48078) ^e (47724)	(676) ^f		$[0.6032]$ $[0.6005]$		[2.5]	$[1.849_4]$	D \rightarrow A, R	31830.74 Z 31810.39 Z	(3)*
C $^2\Pi_r$	39041.2 38925.8	892.6 ₄	H 6.74	$[0.7052]^g$ $[0.6998]$	h		$[1.711_8]$	C \rightarrow X, R γ -bands	38897.28 Z 38781.93 Z	(1)*
B $^2\Sigma^+$	36223.4	770	H 4.0	$[0.6311]^i$	h	[1.53]	$[1.806_0]$	B \rightarrow A, V β -bands	20022.84 Z 20354.99 Z	(1)* (2)(3)*

BrF, BrF⁺:

^aFrom the heats of formation (7) of BrF and Br₂ and the dissociation energies of Br₂ and F₂. A higher value, 2.71 eV, was suggested (11) on the basis of an assumed 20 % failure for the linear Birge-Sponer extrapolation of the ground state.

^bFrom the photoelectron spectrum (9); in reasonable agreement with an electron impact appearance potential of 11.8 eV (5).

^c $\omega_e y_e = -0.22$.

^dFragmentary observations; the constants are very uncertain. See (11).

^eRotational constants recalculated by (6) from (1).

^f $\mu_{el} = 1.29$ D; also values for eqQ(^{79,81}Br). Zeeman effect (10).

^gD₀⁰(BrF) + I.P.(Br) - I.P.(BrF).

^hFrom the photoelectron spectrum (9).

(1) Smith, Tidwell, Williams, PR 77, 420 (1950).

(2) Durie, PRS A 207, 388 (1951).

(3) Brodersen, Sicre, ZP 141, 515 (1955).

(4) Brodersen, Mayo, ZP 143, 477 (1955).

(5) See ref. (6) of BrCl.

(6) Calder, Ruedenberg, JCP 49, 5399 (1968).

(7) See ref. (10) of BrCl.

(8) Clyne, Coxon, Townsend, JCS FT II 68, 2134 (1972).

(9) DeKock, Higginson, Lloyd, Breeze, Cruickshank, Armstrong, MP 24, 1059 (1972).

(10) Ewing, Tigelaar, Flygare, JCP 56, 1957 (1972).

(11) Coxon, CPL 33, 136 (1975).

BrO: ^aFrom the near-convergence of the absorption bands A ← X₁ assuming dissociation of A into Cl(²P_{3/2}) + O(¹D₂); see (2).

^bNormal isotopic mixture. The vibrational numbering in

BrO (continued):

neither A nor X₁ is quite certain. In order to fit the absorption and the emission bands into the same vibrational scheme it was assumed (2) that the longest-wavelength absorption band was 1-0 and that the v" numbering of the emission bands (1) had to be raised by four units.

^c $\omega_e y_e = -0.074$.

^dAll A ← X₁ bands are diffuse on account of predissociation, though a few bands show evidence of rotational fine structure.

^eA₀ = - 815 from EPR sp. (5); (8) estimate A₀ = - 980.

^fEffective constants.

^gFrom the "true" B_e = 0.4299 (7).

^h $\mu_{el}(v=0) = 1.765$ D (7); 1.61 D from Stark effect in the gas-phase EPR sp. (3)(6). For eqQ(^{79,81}Br) and magnetic hyperfine parameters for both isotopes see (4)(5)(7)(8).

(1) Coleman, Gaydon, DFS 2, 166 (1947).

(2) Durie, Ramsay, CJP 36, 35 (1958).

(3) Carrington, Levy, Miller, JCP 47, 3801 (1967).

(4) Powell, Johnson, JCP 50, 4596 (1969).

(5) Carrington, Dyer, Levy, JCP 52, 309 (1970).

(6) Byfleet, Carrington, Russell, MP 20, 271 (1971).

(7) Amano, Yoshinaga, Hirota, JMS 44, 594 (1972).

(8) Brown, Byfleet, Howard, Russell, MP 23, 457 (1972).

BS: ^aThermochemical value (mass-spectrom.)(5). Different values suggested by (4).

^bSpin-splitting constant $\gamma_0 = +0.0245$.

^cA₀ = - 321.53.

^d $|\Delta v_{fe}| = 0.0197(J+\frac{1}{2})$.

^eA₀ = - 175.05.

^fEstimated from the observed isotope shift for the 0-0

^g $\Delta v_{fe} \approx +0.01(J+\frac{1}{2})$.

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band.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{11}\text{B}^{32}\text{S}$ (continued)											
A $2\Pi_i$	16209.7 ^j 15876.0	753.61	H	4.67	[0.6209] ^k [0.6185]	0.0059 ^l	[1.69]	1.818 ₂	A \rightarrow X, R α -bands	16002.2 H 15996.8 H 15668.5 H 15663.1 H ESR sp. ^o . <u>Ab initio</u> calc. (8)	(1)* (6)
X $2\Sigma^+$	0	1180.17	H	6.31 ^m	0.7948 ₉ ⁿ	0.0060 ₅ ^l	[1.40]	1.6092			
$^{(11)}\text{B}^{(80)}\text{Se}$		$(\mu = 9.6762979_4)$ $D_0^0 = 4.7_5 \text{ eV}^a$								JUN 1976	
$^{(11)}\text{B}^{(28)}\text{Si}$		$(\mu = 7.9003924_8)$ $D_0^0 = 2.9_5 \text{ eV}^a$								JUN 1976	
$^{12}\text{C}_2$		$\mu = 6.00000000$ $D_0^0 = 6.21 \text{ eV}^a$ I.P. = 12.15 eV ^b Theoretical work and potential functions (16)(29)(35)(49).								JUL 1976 A	
F $1\Pi_u$	[75456.9]	[1557.5]	Z		1.645	0.019	6	1.307	F \leftarrow X, R	74532.9 Z	(51)*
g $3\Delta_g$	[73183.6] ^c	[1458.06]	Z		1.5238	0.0170	6.6	1.3579	g \leftarrow a, R	71649.6 Z	(51)*
f $3\Sigma_g^-$	71045.8	1360.5	Z	14.8	1.448 ^d	0.040 ^e	10	1.393	f \leftarrow a, R	70188.4 Z	(51)*
E $1\Sigma_g^+$	55034.7	1671.5 ₀	Z	40.02 ^f	1.7897	0.0387 ^g	8.3 ^h	1.2529	E \rightarrow A, ⁱ V	46668.3 Z	(10)*
D $1\Sigma_u^+$	43239.4 ₄	1829.57	Z	13.94	1.8332 ^j	0.0196	7.32 ^j	1.2380	D \leftrightarrow X, ^k Mulliken b.	43226.7 ₄ ^j Z	(2)* (11) (46)
e $3\Pi_g$	40796.65 ^l	1106.56	Z	39.260 ^m	1.1922	0.0242	6.3 ⁿ	1.5351	e \rightarrow a, ^o R Fox-Herzberg b.	39806.46 Z	(7)*
C' $1\Pi_g$		Preliminary constants from perturbations in C $1\Pi_g$; see (40).									
C $1\Pi_g$	34261.3	1809.1	Z	15.81 ^p	1.7834	0.0180 ^p	6.8	1.2552	C \rightarrow A, ^q V _R Deslandres-d'Azambuja b.	25969.19 Z	(1)(3)(8) (50)
d $3\Pi_g$	20022.50 ^r	1788.22	Z	16.440 ^s	1.7527 ^t	0.01608 ^u	6.7 ₄ ^v	1.2661	d \leftrightarrow a, ^w V _R Swan b. (d \leftarrow X) ^x	19378.44 Z	(6)* (25) (42)* (48)
c $3\Sigma_u^+$	13312.1	1961.6 ^y		13.7	1.87 ^y			1.23			

BS (continued):

^h $v=1$ of $C\ ^2\Pi_r$ interacts with $v=5$ of $B\ ^2\Sigma^+$ and with an unidentified state; see (3).

ⁱSpin splitting constant $\gamma_0 = -0.0901$.

^j $A_0 = -330.91$ (from $B \rightarrow A$).

^k $\Delta v_{fe} = +0.0176(J+\frac{1}{2})$.

^lPerturbations between higher levels of $A\ ^2\Pi_i$ and of $m_w v_e = -0.004$ (3). | $x\ ^2\Sigma^+$; see (3).

ⁿSpin splitting constant $\gamma = +0.013$ (7).

^oIn inert matrices (Ne, Ar) at 4 K (7).

(1) Zeeman, CJP 29, 336 (1951).

(2) Koryazhkin, Maltsev, VMUK No. 4, 92 (1968).

(3) McDonald, Innes, JMS 29, 251 (1969).

(4) Gingerich, CC (1970), p. 580.

(5) Uy, Drowart, HTS 2, 293 (1970).

(6) Singh, Tewari, Mohan, IJPAP 2, 269 (1971).

(7) Brom, Weltner, JCP 57, 3379 (1972).

(8) Ball, Thomson, CPL 36, 6 (1975).

BSe: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (5) of BS.

BSi: ^aThermochemical value (mass-spectrom.)(1).

(1) Verhaegen, Stafford, Drowart, JCP 40, 1622 (1964).

C_2 : ^aAverage of thermochemical values (15)(55). Smaller values of 6.07 and 6.11 eV have been derived on the basis of a somewhat doubtful extrapolation of the vibrational levels in $d\ ^3\Pi_g$ (39) and of an extrapolated limiting curve of the $C\ ^1\Pi_g$ state (41). See also (13).

^bFrom photoionization and heat of formation of C_2N_2 (38).

^c $A_0 = -8.8 + 0.020 J$; $A_1 = -7.4$.

^dSpin splitting constant $\lambda \approx 0.41$.

^e $v_e = +0.006$.

C_2 (continued):

^f $w_e y_e = +0.248$.

^g $\gamma_e = -0.00055$. Rotational constants re-evaluated; (10) gives

^h $\beta_e = +0.6 \times 10^{-6}$. | $B_e = 1.7930$, $\alpha_e = 0.0421$.

ⁱFranck-Condon factors (30); electronic trans. moment (57).

^jFrom (46); slightly different constants in (2). $\beta_e \approx 3 \times 10^{-8}$.

^kRadiative lifetime $\tau = 14.6$ ns, $f_{00} = 0.055$ (53). The corresponding electronic transition moment is in only moderate agreement with (57). Franck-Condon factors (14)(30).

^lA not determined, but much smaller than for a $^3\Pi_u$.

^m $w_e y_e = +2.8050$, $w_e z_e = -0.1271$.

ⁿ $\beta_e = +0.29 \times 10^{-6}$.

^oFranck-Condon factors (14)(20)(30); el. trans. moment (57).

^pThe AG and B_v curves are irregular (9)(40) and cannot be represented by the constants given without the use of higher order terms. The perturbation is strongest near $v=5$. Breaking-off at high J observed (41) in $v=0,1,2$.

^qFranck-Condon factors (14)(30); el. trans. moment (57).

^r $A = -16.9$.

^s $w_e y_e = -0.5067$. (52) have observed bands up to $v'=14$.

^tNumerous small perturbations by higher levels of $b\ ^3\Sigma_g^-$ (19) and $x\ ^1\Sigma_g^+$ (47) and by unidentified states.

Swan bands emitted in low-pressure oxy-acetylene flames show a distinct intensity alternation ascribed to excitation by collisions with $c\ ^3\Sigma_u^+$ carbon molecules (24)(34).

Under certain conditions in discharges through CO the $v'=6$ progression of the Swan system appears almost exclusively and was at one time considered as a separate band system, the so-called high-pressure bands of carbon (5)(36)(45)*. Isotope studies (44) leave no doubt that the high-pressure bands are the $v'=6$ progression of the Swan system.

(continued p. 114)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}_2$ (continued)										
A $^1\Pi_u$	8391.00	1608.35	Z 12.07 ₈ ^z	1.6163 ₄ ^{a'}	0.0168 ₆ ^z	6.44 ^z	1.3184 ₃	A \leftrightarrow X, ^{b'} R 8268.16	Z	(18)
b $^3\Sigma_g^-$	6434.2 ₇	1470.4 ₅	Z 11.1 ₉ ^{c'}	1.4985 ₂ ^{d'}	0.0163 ₄ ^{e'}	6.22	1.3692 ₈	Phillips b.		
a $^3\Pi_u$	716.2 ₄ ^{g'}	1641.35	Z 11.67	1.6324 ₆ ^{h'}	0.01661	6.44	1.3119 ₀	b \rightarrow a, ^{f'} R 5632.7	Z	(17)*
X $^1\Sigma_g^+$	0	1854.71	Z 13.34 ₀ ^{i'}	1.8198 ₄	0.0176 ₅ ^{i'}	6.92 ^{i'}	1.2425 ₃	Ballik-Ramsay b.		

C_2 (continued):

$$\begin{aligned} u\gamma_e &= -0.001274. \\ v\beta_e &= +0.103 \times 10^{-6}. \end{aligned}$$

^wRadiative lifetime $\tau = 170$ ns (53), in reasonable agreement with (37) but much shorter than (22). f values obtained from the lifetime measurements as well as by other methods (28)(31)(32)(43) have been reviewed in (56). The latter authors' expression for the r dependence of the electronic transition moment was placed on an absolute scale using an average $f_{00} = 0.020$. For a more recent measurement of the electronic transition moment see (57). Franck-Condon factors (14)(20)(21)(27)(30).

^xIn solid matrices; tentative assignment by (23) who also report the observation of $d \leftarrow a$. See, however, (33).

^yFrom perturbations in A $^1\Pi_u$ (18).

$$\left. \begin{aligned} z w_e y_e &= -0.010; \\ \gamma_e &= -0.000054; \\ \beta_e &= +0.036 \times 10^{-6}. \end{aligned} \right\} \begin{array}{l} \text{Very slightly revised constants in} \\ (54) \text{ based on the same data.} \end{array}$$

^{a'} Λ -type doubling, $\Delta v_{ef} = -0.00023 \times J(J+1)$. Perturbations by $c^3\Sigma_u^+$.

^{b'} $f_{00} = 0.0025$; see (59) for a comparison with other absolute measurements. Reasonably consistent with the electronic transition moment obtained by (57). Franck-Condon factors (14)(21)(27)(30).

^{c'} $w_e y_e = +0.028$ (19).

^{d'}Spin-splitting parameters $\lambda_0 = 0.11$, $\gamma_0 = -0.0036_5$ (58). Small perturbations by levels of X $^1\Sigma_g^+$ (17).

^{e'} $\gamma_e = -0.000087$ (19).

^{f'}Franck-Condon factors (30); electronic transition moment (57).

^{g'}A = -15.25; (58) gives additional spin-coupling constants.

^{h'} Λ -type doubling; see (17) and (58).

^{i'} $\left. \begin{aligned} w_e y_e &= -0.172; \\ \gamma_e &= -0.00023; \\ \beta_e &= +0.081 \times 10^{-6}. \end{aligned} \right\} \begin{array}{l} \text{From (18); very slightly revised con-} \\ \text{stants in (54) based on the same data.} \end{array}$

C₂ (continued):

- (1) Dieke, Lochte-Holtgreven, ZP 62, 767 (1930).
- (2) Landsverk, PR 56, 769 (1939).
- (3) Herzberg, Sutton, CJR A 18, 74 (1940).
- (4) Gerß, Schmid, PR 62, 82 (1942).
- (5) Herzberg, PR 70, 762 (1946).
- (6) Phillips, ApJ 108, 434 (1948).
- (7) Phillips, ApJ 110, 73 (1949).
- (8) Herzberg, MOLSPEC 1 (1950).
- (9) Phillips, ApJ 112, 131 (1950).
- (10) Freymark, AP(Leipzig) 8, 221 (1951).
- (11) Norrish, Porter, Thrush, Nature 169, 582 (1952).
- (12) Nicholls, PPS A 69, 741 (1956).
- (13) Drowart, Burns, DeMaria, Inghram, JCP 31, 1131 (1959).
- (14) Nicholls, Fraser, Jarman, CF 3, 13 (1959).
- (15) Brewer, Hicks, Krikorian, JCP 36, 182 (1962).
- (16) Read, Vanderslice, JCP 36, 2366 (1962).
- (17) Ballik, Ramsay, ApJ 137, 61 (1963).
- (18) Ballik, Ramsay, ApJ 137, 84 (1963).
- (19) Callomon, Gilby, CJP 41, 995 (1963).
- (20) Jain, JQSRT 4, 427 (1964).
- (21) Ortenberg, OS(Engl. Transl.) 16, 398 (1964).
- (22) Jeunehomme, Schwenker, JCP 42, 2406 (1965).
- (23) Barger, Broida, JCP 43, 2371 (1965).
- (24) Bleekrode, Nieuwpoort, JCP 43, 3680 (1965);
Nieuwpoort, Bleekrode, JCP 51, 2051 (1969).
- (25) Bugrim, Lyutyi, Rossikhin, Tsikora, OS(Engl. Transl.)
19, 292 (1965).
- (26) Mentall, Nicholls, PPS 86, 873 (1965).
- (27) Spindler, JQSRT 5, 165 (1965).
- (28) Fairbairn, JQSRT 6, 325 (1966).
- (29) Fougere, Nesbet, JCP 44, 285 (1966).
- (30) Halmann, Laulicht, ApJ(Suppl.) 12, 307 (1966); JCP
44, 2398 (1966).
- (31) Harrington, Modica, Libby, JCP 44, 3380 (1966).
- (32) Sviridov, Sobolev, Novgorodov, Arutyunova, JQSRT 6, 337,
875 (1966).
- (33) Weltner, McLeod, JCP 45, 3096 (1966).
- (34) Bleekrode, PRR(Suppl.) No. 7 (1967).
- (35) Verhaegen, Richards, Moser, JCP 46, 160 (1967).
- (36) Kunz, Harteck, Dondes, JCP 46, 4157 (1967).
- (37) Fink, Welge, JCP 46, 4315 (1967).
- (38) Dibeler, Liston, JCP 47, 4548 (1967).
- (39) Messerle, Krauss, ZN 22 a, 1744 (1967).
- (40) Messerle, Krauss, ZN 22 a, 2015 (1967).
- (41) Messerle, Krauss, ZN 22 a, 2023 (1967).
- (42) Tyte, Innanen, Nicholls, IAMS 5 (1967).
- (43) Arnold, JQSRT 8, 1781 (1968).
- (44) Dhumwad, Narasimham, CJP 46, 1254 (1968).
- (45) Meinel, Messerle, ApJ 154, 381 (1968).
- (46) Messerle, ZN 23 a, 470 (1968).
- (47) Phillips, JMS 28, 233 (1968).
- (48) Phillips, Davis, BAMS 2 (1968).
- (49) Verhaegen, JCP 49, 4696 (1968).
- (50) Cisak, Dabrowska, Rytel, APP 36, 497 (1969).
- (51) Herzberg, Lagerqvist, Malmberg, CJP 47, 2735 (1969).
- (52) Kini, Savadatti, JP B 2, 307 (1969).
- (53) Smith, ApJ 156, 791 (1969).
- (54) Marenin, Johnson, JQSRT 10, 305 (1970).
- (55) Kordis, Gingerich, JCP 58, 5058 (1973).
- (56) Danylewych, Nicholls, PRS A 339, 197, 213 (1974).
- (57) Cooper, Nicholls, JQSRT 15, 139 (1975).
- (58) Veseth, CJP 53, 299 (1975).
- (59) Roux, Cerny, d'Incan, ApJ 204, 940 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{12}\text{C}_2^+$										
A $2\Sigma_g^-$ (40143)		$\mu = 5.99986286$		$D_0^0 = 5.32 \text{ eV}^a$						JUL 1976
(X) $2\Pi_u$ ^d 0 ^e		(1340)		$[1.648]^b$		[100]	[1.306]	A \leftarrow X, ^c	40137.8 Z	(2)*
		(1350)		$[1.659]$		[100]	[1.301]			
$^{12}\text{C}_2^-$										
a $4\Sigma_u^+$ (19448)		$\mu = 6.00013715$		$D_0^0 = 8.48 \text{ eV}^a$		I.P. = 3.54 eV^b				JUL 1976 A
B $2\Sigma_u^+$ 18390.88		(1074) ^c (25)		$(1.135)^c$ (0.0035)			(1.573)	B \leftrightarrow X, ^h V	18483.98 Z	(1)*
A $2\Pi_u$		1968.73 Z 14.43 ₃ ^d		1.8774_5^e 0.0177 ₆ ^f		68.4 ^g	1.2233 ₀	A \leftarrow X,		(7)
X $2\Sigma_g^+$ 0		Fragments of absorption bands.								
		1781.04 Z 11.58 ₅ ⁱ		1.7468_5 0.0167		66.9	1.2682 ₁			
$^{40}\text{Ca}_2$										
		$\mu = 19.9812961$		$D_0^0 = 0.12_9 \text{ eV}^a$						JUL 1976 A
		A band system in the region $16100 - 16900 \text{ cm}^{-1}$ and assigned to Ca_2 by (3) is in all probability the same as that usually ascribed to CaO . ^b								
		Emission continuum from 19500 to 25000 cm^{-1} .								(1)
A $1\Sigma_u^+$ ≤ 18963.7		$\geq 136.66^c$ Z	0.716_6^d	$\geq 0.058247^c$	0.0003104^e	0.459^f	≤ 3.8058	A \leftarrow X, ^g V	18999.7 ^h Z	(2)(4)*
X $1\Sigma_g^+$ 0		64.92 ₈ Z	1.065_1^i	0.046113	0.000702_8^j	0.95_2^k	4.2773			
$^{40}\text{Ca}^{79}\text{Br}$										
		$\mu = 26.5289081$		$D_0^0 = 3.2_8 \text{ eV}^a$						JUL 1976 A
H 36798.7		343.4 H	1.0					H \rightarrow A, V	20840.2 H 20904.6 H	(5)
E $2\Sigma^+$ 33942.2		318.6 ^b H	1.2					E \rightarrow X, V	33958.8 H	(4)
D $2\Sigma^+$ 31190.8		326.6 ^c H	1.02					D \leftrightarrow X, V	31211.4 H	(2)(4)

$$C_2^+: a_{D_0^0}(C_2) + I.P.(C) - I.P.(C_2).$$

^bPerturbations.

^cIt is not entirely certain that the absorption spectrum obtained in flash discharges through C_2H_2/He mixtures is due to C_2^+ .

^dNot certain that this is the ground state. Theoretical calculations (1) suggest that $^2\Pi_u$ lies at 0.7 eV above the predicted $^4\Sigma_g^-$ ground state.

$$^e A_0 = -8.0 \text{ cm}^{-1}.$$

(1) Verhaegen, JCP 49, 4696 (1968).

(2) Meinel, CJP 50, 158 (1972).

$$C_2^-: a_{D_0^0}(C_2) \text{ and the electron affinities of } C_2 \text{ and of } C (=1.268 \text{ eV}).$$

^bPhotodetachment threshold (3).

^cConstants derived (11) from the perturbations (1) in $B^2\Sigma_u^+$. Ab initio calculations by (9) and (10) independently predict the existence of a $^4\Sigma_u^+$ state slightly above $B^2\Sigma_u^+$ with r_e and ω_e values near those derived from the perturbations.

$$^d \omega_e \nu_e = -0.324.$$

^eSmall perturbations by a $^4\Sigma_u^+$.

$$^f \gamma_e = -0.00037$$

$$^g + [1.0(v+\frac{1}{2}) + 0.08(v+\frac{1}{2})^2] \times 10^{-7}.$$

^hThe spectrum was observed in flash discharges in CH_4 (1), behind reflected shock waves [$f_{el} \approx 0.017$ (8)], and in rare gas matrices (2)(4)(6)(11)(12). Conclusive proof that it belongs to C_2^- was supplied by two-photon photodetachment spectroscopy (7). Franck-Condon factors (5).

$$^i \omega_e \nu_e = -0.027.$$

(1) Herzberg, Lagerqvist, CJP 46, 2363 (1968).

(2) Milligan, Jacox, JCP 51, 1952 (1969).

(3) Feldmann, ZN 25 a, 621 (1970).

(4) Frosch, JCP 54, 2660 (1971).

C_2^- (continued):

(5) Singh, Maheshwari, IJPAP 2, 296 (1971).

(6) Bondybey, Nibler, JCP 56, 4719 (1972).

(7) Lineberger, Patterson, CPL 13, 40 (1972).

(8) Cathro, Mackie, JCS FT II 69, 237 (1973).

(9) Barsuhn, JP B 7, 155 (1974).

(10) Thulstrup, Thulstrup, CPL 26, 144 (1974).

(11) Bondybey, Brus, JCP 63, 2223 (1975).

(12) Brus, Bondybey, JCP 63, 3123 (1975).

Ca_2 : ^aExtrapolation of the vibrational levels in $X^1\Sigma_g^+$.

^bThe B_v values quoted by (3) are of the same order as those for CaO .

^cVibrational numbering unknown.

$$^d - 0.0037_4(v+\frac{1}{2})^3 - 0.000080(v+\frac{1}{2})^4.$$

$$^e - [2.15(v+\frac{1}{2})^2 + 0.097(v+\frac{1}{2})^3] \times 10^{-6}.$$

$$^f H_e = +1.9 \times 10^{-14}.$$

^gRKR curves and Franck-Condon factors (4).

^hEnergy of the lowest observed vibrational level relative to $X^1\Sigma_g^+(v=0)$.

$$^i \omega_e \nu_e = +0.0025_9.$$

$$^j \gamma_e = -0.0000073_5.$$

$$^k + [0.043_1(v+\frac{1}{2}) + 0.0010_7(v+\frac{1}{2})^2] \times 10^{-7}; H_e = -1.4 \times 10^{-13}, \text{ and higher order constants (4).}$$

(1) Hamada, PM 12, 50 (1931).

(2) Weniger, Proc. I. A. U. Colloquium on Late-type Stars, Trieste (1966), edited by M. Hack; p. 25.

(3) Kovalenok, Sokolov, ISOANK No. 4, 118 (1967); IVUZF 11(3), 27 (1968).

(4) Balfour, Whitlock, CJP 53, 472 (1975).

$CaBr$: ^aFlame photometric value (7)(8).

^bNormal isotopic mixture.

^cSlightly different constants in (6).

(continued p. 119)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{40}\text{Ca}^{79}\text{Br}$ (continued)										
C $^2\Pi$	25537.5 25314.0	265.2	H 0.97					$C^d \leftrightarrow X, ^e R$	25527.4 25303.9	H H (2)(10)
B $^2\Sigma^+$	16380.0	284.6	H 0.92					$B^f \leftarrow X, ^g V$	16379.6	H (2)
A $^2\Pi$	15985.8 15922.5	288.1	H 0.92					$A^h \leftrightarrow X, ^i V$	15987.2 15923.9	H H (1)(2)
X $^2\Sigma^+$	0	285.3	H 0.86							
$^{40}\text{Ca}^{35}\text{Cl}$										JUL 1976 A
		$\mu = 18.6496606$		$D_0^0 = 4.0_9 \text{ eV}^a$						
G ($^2\Delta$)	36712 36708	434.0	H ^Q 1.1					$G \rightarrow A, V$	20580 20645	H ^Q H ^Q (6)
F ($^2\Pi$)	35700 35676	432.5	H 0.8 ^b					$F \rightarrow B, V$	18884 18859	H H (6)
E ($^2\Sigma$)	34266.4	413.3	1.68					$F \rightarrow A, V$	19567 19612	H H (6)
D ($^2\Sigma$)	31107.8	423.4	1.61					$E \rightarrow B, V$	17439.8	H (11)
C $^2\Pi_r$	26574.6 26498.9	[333.86] 336.0	Z H 1.4 H					$E \leftarrow X, V$	34288.1	(5)
B $^2\Sigma^+$	16849.4	366.7 ^e	H 1.4 ₃					$D \leftarrow X, V$	31134.5	(5)
A $^2\Pi$	16163.2 16093.7	372.3	H 1.2 ⁱ					$C^d \leftrightarrow X, R$	26557.80 26481.82	Z Z (1)(3)(7)
X $^2\Sigma^+$	0	[367.53]	Z 1.31 H					$B^g \leftrightarrow X, ^h V$	16847.6	H (1)(2)(3) (14)*
								$A^j \leftrightarrow X, V$	16164.3 16094.8	H ^Q H ^Q (1)(2)(3)
$^{40}\text{Ca}^{19}\text{F}$										JUL 1976
		$\mu = 12.8767412$		$D_0^0 = 5.4_8 \text{ eV}^a$						
F $^2\Pi$	37547.8	681.7	H 3.55					$F \leftrightarrow X, V$	37595.1	H (4)(8)
E $^2\Sigma^+$	34134.6	646.3	H 3.24					$E \leftrightarrow X, V$	34164.4	H (4)* (8)
D $^2\Sigma^+$	30771.9	650.7	H 2.89					$D \leftarrow X, V$	30803.9	H (4)*
C $^2\Pi$	30284.4 30255.1	481.7	H 2.02					$C \leftrightarrow X, R$	30232.1 30202.8	H H (1)(4)*

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{40}\text{Ca}^{19}\text{F}$ (continued)											
B $^2\Sigma^+$	18844.5	566.1 ^b	2.80	$[(0.336_1)]^c$				$B^d \leftrightarrow X, ^e R$	18834.2 (Z)	(1)(2)*	
A $^2\Pi_r$	16562.3 ^f 16489.8	593.4 [586.8]	H^g Z	3.113 ^g 3.427 ^h	0.3436^{ij}	0.0028	(4.6)	1.952	$A^k \leftrightarrow X, \nu_R$	16565.6 Z 16493.1 Z	(1)(2)* (9) (12)
X $^2\Sigma^+$	0	[581.1]	Z	2.74 H	0.338_5	0.0026	(4.5)	1.967	ESR sp. ^l		

CaBr (continued):

- ^dRadiative lifetime $\tau(v=0,1) = 32.5$ ns (9).
^eFour heads.
^fRadiative lifetime $\tau(v=0) = 42.9$ ns (9).
^gDouble heads on account of large spin doubling in the upper state. Constants refer to the short-wavelength head.
^hRadiative lifetime $\tau(v=1) = 34.0$ ns (9). | head.
ⁱFour heads. For a reproduction of the spectrum see Fig. 1e of (3) who wrongly attributed the spectrum to MnBr.
 (1) Hedfeld, ZP 68, 610 (1931).
 (2) Harrington, Dissertation (U. of California, 1942).
 (3) Hayes, Nevin, PPS A 68, 665 (1955).
 (4) Reddy, Rao, IJPAP 6, 181 (1968).
 (5) Reddy, Reddy, Rao, CS 39, 485 (1970).
 (6) Shah, IJPAP 8, 118 (1970).
 (7) Gurvich, Ryabova, Khitrov, FSCS No. 8, 83 (1973).
 (8) Khitrov, Ryabova, Gurvich, HT(USSR) 11, 1005 (1973).
 (9) Dagdigian, Cruse, Zare, JCP 60, 2330 (1974).
 (10) Joshi, Gopal, Pramāṇa 4, 276 (1975).

CaCl: ^aThermochemical value (mass-spectrom.)(8)(9); in good agreement with flame photometric results (10)(12).
^b $w_e y_e = +0.06$.

CaCl (continued):

- ^c Λ -type doubling (7).
^dRadiative lifetime $\tau(^2\Pi_{3/2}, v=0) = 25.0$ ns (13).
^eRecalculated from the heads of the 0-0 sequence of B-X, using for the ground state the constants given in the Table. In good agreement with constants derived from E-B.
^fThe predissociation above $v=15$ reported by (4) is not compatible with a dissociation energy of more than 4 eV.
^gRadiative lifetime $\tau(v=0) = 38.2$ ns (13).
^hDouble heads on account of g-type doubling in the upper state. The constants refer to the short-wavelength head.
ⁱ $w_e y_e = -0.05$. Average of the constants from F-A and G-A. Considerably different constants are obtained from A-X owing to large head-origin separations.
^jRadiative lifetime $\tau(v=2) = 28.9$ ns (13).
 (1) Walters, Barratt, PRS A 118, 120 (1928).
 (2) Asundi, PIAS A 1, 830 (1935).
 (3) Parker, PR 47, 349 (1935).
 (4) Hellwege, ZP 100, 644 (1936).
 (5) See ref. (2) of CaBr.
 (continued p. 121)

CaF: See p. 121.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{40}\text{Ca}^1\text{H}$										
		$\mu = 0.98303388$		$D_0^0 \leq 1.70 \text{ eV}^a$		$I.P. = 5.86 \text{ eV}^b$				JUL 1976 A
I ($^2\Sigma$)				[(4.60)]			[(1.93)]	I \leftarrow X,	(39477)	(14)
H ($^2\Sigma$)				[(4.41)]			[(1.97)]	H \leftarrow X,	(38798)	(14)
F $^2\Sigma^+$	36705	1487 ^c	28	[4.6867]		[2.017]	[1.9128]	F \leftarrow X, V	36797.05 Z	(11)(12)* (14)
M $^2\Delta$	} (4d) e (34735)	[1458] ^f		[4.89] ^d	0.113 ₉ (0.085)	[2.8] ^d [1.17] ^d	[1.87]	M \leftarrow X,	35481.8 ^d	(22)*
J $^2\Pi$				[4.898] ^d			[1.87 ₁]	J \leftarrow X,	35068.5 ₃ ^d	(22)*
G $^2\Sigma^+$				[4.765] ^d			[1.897]	G \leftarrow X,	34819.5 ^d	(22)*
L $^2\Pi$	} (5p) (32680) ^g	[1407.6] ^h	[1391] ^h	[4.620 ₄] ^h	0.113 ₉ (0.085)	[1.92 ₀] ^{hi}	1.914 ₈	L \leftarrow X,	32739.3 ₇ ^h	(21)*
K $^2\Sigma^+$				[4.601] ^{hj}		[1.93] ^{hk}	1.922	K \leftarrow X,	32691.1 ^h	(21)*
C $^2\Sigma^+$	28276	1445	H 25	[4.58] ^{lm}		[1.7] ^l	[1.94]	C \leftrightarrow X, V	28348.0 ^l	(1)* (4)* (7)
D $^2\Sigma^+$	22602	1150	Z 33.0	2.50 ⁿ	0.01		2.62	D \rightarrow X, R	22524 Z	(4)(6)
E $^2\Pi$	20418 ^o	1248.6	H ^q 21.8	[4.284]		[2.2]	[2.001]	E \rightarrow X, ^p V	20392 Z	(9)

Ca^1H : ^aFrom the predissociation in C $^2\Sigma^+$, assuming dissociation into $\text{Ca}(^3\text{P}) + \text{H}(^2\text{S})$.

^bFrom the observation of Rydberg states in the absorption spectrum (22).

^cFrom isotope relations (12).

^dDeperturbed constants for the three interacting states which form the d complex. The $^2\Delta_{5/2}$ component was not observed. Most of the lines are somewhat diffuse. The $^2\Pi - ^2\Sigma$ band whose low J lines are sharp had been misinterpreted by (20) in terms of two overlapping $^2\Sigma - ^2\Sigma$ transitions. Small local perturbations.

^e $A_0 = +5.0$.

^fFrom the proposed assignment of the 1-0 band by (14). (22) observe a diffuse single branch only.

^g $A_0 = +18.8$, $A_1 = +19.3$.

^hDeperturbed constants for the two interacting states which form the p complex. Small local perturbations.

ⁱ $D_1 = 2.06_4 \times 10^{-4}$; $H_0 = +4.7 \times 10^{-9}$.

^j F_1 levels not observed, presumably on account of predissociation. In $v=1$ both spin components seem to be predissociated.

^k $H_0 = +2.5 \times 10^{-9}$.

Ca¹H (continued):

^lConstants derived from high N values. At low N, v=0 is perturbed by a state of smaller B value. The observed origin of the 0-0 band is at 28352.5 cm⁻¹.

^mAt low pressure predissociation above v=0, N=10.

ⁿStrong perturbations for higher N values.

^oA ≈ 9.3.

^pTwo Q heads.

(continued p.123)

CaCl (continued):

(6) Schütte, ZN 2 a, 891 (1954).

(7) Morgan, Barrow, Nature 185, 754 (1960).

(8) Zmbov, CPL 4, 191 (1969).

(9) Hildenbrand, JCP 52, 5751 (1970).

(10) See ref. (7) of CaBr.

(11) Khanna, Dubey, IJPAP 11, 510 (1973); 13, 603 (1975).

(12) Ryabova, Khitrov, Gurvich, HT(USSR) 10, 669 (1973).

(13) See ref. (9) of CaBr.

(14) Darji, Shah, IJPAP 13, 187 (1975).

CaF: ^aThermochemical value (mass-spectrom.)(5)(7); 5.8₅ eV by flame photometry (6).

^bRecalculated from the heads of the 0-0 sequence using for the ground state the constants given in the table.

^cUsing data from (2) and (12).

^dRadiative lifetime τ(v=0) = 25.1 ns (11).

^eDouble heads on account of large spin-doubling in the upper state and high N values of the heads.

^fA₀ = + 73.4.

^g_wy_e = + 0.0051.

CaF (continued):

^h_wy_e = + 0.0619.

ⁱΛ-type doubling in 2Π_{1/2}, Δv_{fe} = - 0.045(J+½).

^jThe possibility of predissociation above v=16, as suggested by (3), is now ruled out by the new value for D₀⁰.

^kRadiative lifetime τ(v=0) = 20.2 ns (11).

^lIn rare gas matrices at 4 K (10).

(1) Johnson, PRS A 122, 161 (1926).

(2) Harvey, PRS A 133, 336 (1931).

(3) See ref. (4) of CaCl.

(4) Fowler, PR 52, 645 (1941).

(5) Blue, Green, Bautista, Margrave, JPC 62, 877 (1963).

(6) Ryabova, Gurvich, HT(USSR) 2, 749 (1964).

(7) Hildenbrand, Murad, JCP 44, 1524 (1966).

(8) Prasad, Narayan, IJP 43, 205 (1969).

(9) Subbaram, Rao, IJP 43, 312 (1969).

(10) Knight, Easley, Weltner, Wilson, JCP 54, 322 (1971).

(11) See ref. (9) of CaBr.

(12) Field, Harris, Tanaka, JMS 52, 107 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References					
								Design.	v_{00}						
$^{40}\text{Ca}^1\text{H}$ (continued)															
B	$2\Sigma^+$	15762 (4p)	1285	20	[4.3410] ^q	0.116	[2.020] ^{qr}	1.974 ₄	B \leftrightarrow X, v	15754.96 ^q	(2)(3)(8)* (15)(23)(24)				
A	$2\Pi_r$								14413 ^s	1333		20	[4.3476] ^q	0.106	[1.883] ^{qt}
X	$2\Sigma^+$	0	1298.34	Z	19.10	4.2766 ^u	0.0970	1.837 ^v	2.0025	ESR sp. ^w					
$^{40}\text{Ca}^2\text{H}$											JUL 1976 A				
		$\mu = 1.91746270$		$D_0^0 \leq 1.72 \text{ eV}^a$											
F	$2\Sigma^+$	(36698) (4d)	[1036.1]	Z	14 ^b	2.434	0.051	[0.49] ^c	1.901	F \leftarrow X, v	36771.40	Z	(3)(4)(5)		
M	2Δ					d									
J	2Π					d							J \leftarrow X,	35034.16 ^e	(8)
G	$2\Sigma^+$					d							G \leftarrow X,	(34750)	(8)(4)
L	2Π	(32647) ^f (5p) (32615)	[1020.57] ^g	(15.9)	[2.3830] ^g	0.0412	[0.5018] ^{gh}	1.9125	L \leftarrow X,	32713.61 ^g	(8)				
K	$2\Sigma^+$								[(1012)] ^g	[2.3751] ^{gi}	(0.019)	[0.503] ^g	1.920	K \leftarrow X,	32665.5 ^g
C	$2\Sigma^+$				[(2.35)] ^j		[(0.44)]	[(1.93)]	C \rightarrow X, v	28322	Z	(1)* (2)*			
B	$2\Sigma^+$				2.282 ^k	0.045	[0.54] ^l	1.963	B \rightarrow X, v	15748.8	Z	(2)			
X	$2\Sigma^+$	0	[910.4]	Z		[2.1769] ^m	0.035	[0.479] ⁿ	2.001 ₆						
CaH^+								The spectrum of CaH^+ reported in the previous edition (MOLSPEC 1) is in fact due to MgH .							

Ca¹H (continued):

^qDeperturbed constants for the strongly interacting states A ² Π and B ² Σ^+ ; see (23). For an extensive discussion of the rotational structure of the two states (including spin and Λ -type doubling) see also (17)(18)(19).

$$r_{H_0} = + 4.31 \times 10^{-9}.$$

$$s_{A_0} = + 79.01; \text{slight } J \text{ dependence (23). See also (17).}$$

$$t_{H_0} = + 5.08 \times 10^{-9}.$$

$$u \text{ Spin-splitting constant } \gamma_v = + 0.042_9 - 0.0010(v + \frac{1}{2}).$$

$$v_{H_e} = + 5.51 \times 10^{-9}.$$

^wIn Ar matrix at 4 K (16).

- (1) Mulliken, PR 25, 509 (1925).
- (2) Hulthén, PR 29, 97 (1927).
- (3) Watson, Bender, PR 35, 1513 (1930).
- (4) Grundström, ZP 62, 235 (1931).
- (5) Mulliken, Christy, PR 38, 87 (1931).
- (6) Grundström, ZP 75, 302 (1932).
- (7) Grundström, ZP 95, 574 (1935).
- (8) Watson, PR 47, 27 (1935).
- (9) Watson, Weber, PR 48, 732 (1935).
- (10) Grundström, Dissertation (Stockholm, 1936).
- (11) Khan, PPS 80, 593 (1962).
- (12) Edvinsson, Kopp, Lindgren, Åslund, AF 25, 95 (1963).
- (13) Khan, PPS 87, 569 (1966).
- (14) Khan, Afridi, JP B 1, 260 (1968).
- (15) Liberale, Weniger, Physica 41, 47 (1969).
- (16) Knight, Weltner, JCP 54, 3875 (1971).
- (17) Veseth, JMS 38, 228 (1971).
- (18) Veseth, MP 20, 1057 (1971).
- (19) Veseth, MP 21, 287 (1971).
- (20) Khan, Hasnain, NC B 18, 384 (1973).
- (21) Kaving, Lindgren, Ramsay, PS 10, 73 (1974).

Ca¹H (continued):

(22) Kaving, Lindgren, PS 10, 81 (1974).

(23) Berg, Klynning, PS 10, 331 (1974).

(24) Berg, Klynning, AA(Suppl.) 13, 325 (1974).

Ca²H: ^aSee a of Ca¹H.

^bFrom isotope relations.

$$c_{D_1} = 0.30 \times 10^{-4}.$$

^dTerm values, but no constants, determined (8) for $v=0$ of J ² Π and G ² Σ . M ² Δ not observed with certainty. G ² $\Sigma(v=0)$ is perturbed by L ² $\Pi(v=2)$. Smaller local perturbations in J ² Π .

^eQ₁₁($\frac{1}{2}$) line.

$$f_{A_0} = + 19.4_8, A_1 = + 19.3.$$

^gSee h of Ca¹H.

$$h_{D_1} = 0.495 \times 10^{-4}; H_1 = - 1.2_5 \times 10^{-9}.$$

ⁱSee j of Ca¹H.

^jStrong perturbations. Breaking off above $v'=0$, $N'=18$.

^kEffective value. Spin-splitting constant $\gamma \approx - 0.364$, but see (6).

$$l_{D_1} = 0.65 \times 10^{-4}.$$

^mSpin-splitting constant $\gamma_0 = + 0.021_6$.

$$n_{D_1} = 0.61 \times 10^{-4}.$$

(1) Grundström, ZP 92, 171 (1935).

(2) See ref. (8) of Ca¹H.

(3) See ref. (12) of Ca¹H.

(4) See ref. (13) of Ca¹H.

(5) See ref. (14) of Ca¹H.

(6) See ref. (18) of Ca¹H.

(7) See ref. (20) of Ca¹H.

(8) Kaving, Lindgren, PS 13, 39 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{40}\text{Ca}^{127}\text{I}$		$\mu = 30.3920472$ $D_0^0 \geq 2.77 \text{ eV}^a$								JUL 1976
E ($^2\Delta$)	36715.7 36713.3	287.2	H ^Q	0.80				E \rightarrow A, V	21092.8 21149.3	H ^Q H ^Q (12)
D ($^2\Sigma$)	31011.4	256.0	H	0.8				D \leftrightarrow X, V	31019.9	H (1)(8)
C $^2\Pi$	23743.96 23315.51	224.72 229.75	H H	0.530 ^b 0.633				C \leftrightarrow X, R	23736.98 23311.03	H H (1)(3)(5)* (6)*
B $^2\Sigma^+$	15715.2	239.9 ₅	H	0.62				B ^c \leftrightarrow X, V	15715.8 ^d 15712.4 ^d	H H (1)(2)(6)* (10)
A $^2\Pi$	15645.6 15586.2	241.6 ₉ 242.6 ₅	H H	0.83 0.62				A ^e \leftrightarrow X, V	15647.2 15588.4	H H (1)(2)(6)* (10)
X $^2\Sigma^+$	0	238.70	H	0.628						
$^{40}\text{Ca}^{16}\text{O}$		$\mu = 11.4229224_5$ $D_0^0 \geq 4.76 \pm 0.15 \text{ eV}^a$								SEP 1976 A
Progression of absorption bands ($\Delta G \approx 850$) in Kr and Xe matrices, 20000 - 26000 cm^{-1} ; observed for both Ca^{16}O and Ca^{18}O , but not definitely assigned.										(15)
Green system of strong emission bands, 17900 - 18300 cm^{-1} ; only one band (18276 cm^{-1}) analyzed (18).								(B \rightarrow A')		(1)(5)(8)* (18)
Orange system of strong emission bands, 15700 - 16700 cm^{-1} ; no analysis.										(1)(5)(7)* (8)*
C $^1\Sigma^+$	28857.8	560.9	Z	4.0	0.3731 ^b	0.0032	(7)	1.989	C \leftrightarrow X, ^c R	28772.4 Z (4)* (11)
B $^1\Pi$	25991	[574.4]	Z		0.388 ₂ ^{db}	0.005 ₅	(7)	1.950	B \leftrightarrow X, ^e R	25913.0 Z (4)(11)
A $^1\Sigma^+$	11554.8	718.9	Z	2.11	0.4059 ₂ ^f	0.00137	5.4	1.9067	A \rightarrow X, R	11548.8 ₄ Z (3)* (6)* (12)(17)
A' $^1\Pi$	8433	545.7	H	2.54	0.337	0.002 ₁		2.09 ₃	A' \rightarrow X, ^g R	8340 (20)*
a $^3\Pi_1$	(8313) ^h	556		3.3	0.335	0.001 ₅		2.09 ₉		
X $^1\Sigma^+$	0	732.1 ₁	Z	4.8 ₁ ⁱ	0.444 ₅₂	0.00338	6.58 ^j	1.8221	k	

CaI: ^aLower bound from a crossed molecular beam experiment (7); in agreement with the theoretical lower limit of ^b $w_e y_e = -0.083$. | (4).
^cRadiative lifetime $\tau(v=4) = 50.9$ ns (11).
^dDouble heads on account of large spin doubling in $B^2\Sigma$.
^eRadiative lifetime $\tau(v=3,5) = 41.7$ ns (11).
 (1) Walters, Barratt, PRS A 118, 120 (1928).
 (2) Hedfeld, ZP 68, 610 (1931).
 (3) Mesnage, AP(Paris) 12, 5 (1939).
 (4) Krasnov, Karaseva, OS(Engl. Transl.) 19, 14 (1965).
 (5) Murty, Reddy, Rao, JP B 3, 425 (1970).
 (6) Maheshwari, Shukla, Singh, IJPAP 9, 327 (1971).
 (7) Mims, Lin, Herm, JCP 57, 3099 (1972).
 (8) Khanna, Dubey, IJPAP 11, 286 (1973).
 (9) Khanna, Dubey, IJPAP 11, 375 (1973).
 (10) Darji, Vaidya, IJPAP 11, 923 (1973).
 (11) Dagdigian, Cruse, Zare, JCP 60, 2330 (1974).
 (12) Kamalasanan, Shah, CS 44, 805 (1975).

CaO: ^aFrom the $Ca + ClO_2$ chemiluminescence spectrum (21). By contrast, the most recent mass-spectrometric (9)(10) and flame-photometric (16) determinations - corrected, where necessary, for a $^1\Sigma$ ground state - lead to $D_0^0 =$
^bPerturbations. | 4.04 eV.
^c ξ system of (2).
^dValue of B^Q ; $B^{PR} - B^Q = +0.0005$.
^e ϵ system of (2).
^fMany rotational perturbations by $A'^1\Pi$ and a $3\Pi_1$ (3)(17).
^gDirectly observed for $v' > 9$ only; vibrational numbering determined from the perturbations in $A^1\Sigma^+$ (17).
^h $A = -58$, from perturbations in $A^1\Sigma^+$ as are the other constants for this state; see (17).
ⁱThe vibrational constants in the Table are derived from

CaO (continued):

levels with $v \leq 4$ (3)(4). From band heads in the A-X system ($v'' \leq 13$), and accounting for head-origin separations, (12) have derived $w_e = 733.4$, $w_e x_e = 5.28$, $w_e y_e = +0.044$.
^j $\beta_e = +0.03 \times 10^{-7}$.

^kThe question whether this is the ground state was for long in doubt but the observation by (19) of a fundamental frequency of 707 cm^{-1} in a nitrogen matrix seems to settle it; see also (17) and the theoretical work of (14). For computed $^1\Sigma$ ground state properties see (13).

- (1) Lejeune, BSRSL 14, 318 (1945).
- (2) Lejeune, Rosen, BSRSL 14, 322 (1945).
- (3) Hultin, Lagerqvist, AF 2, 471 (1951).
- (4) Lagerqvist, AF 8, 83 (1954).
- (5) Gaydon, PRS A 231, 437 (1955).
- (6) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (7) Rosen, Weniger, CR 248, 1645 (1959).
- (8) Pearse, Gaydon, IDSPEC (1963).
- (9) Colin, Goldfinger, Jeunehomme, TFS 60, 306 (1964).
- (10) Drowart, Exsteen, Verhaegen, TFS 60, 1920 (1964).
- (11) Veits, Gurvich, DC 173, 377 (1967).
- (12) Brewer, Hauge, JMS 25, 330 (1968).
- (13) Yoshimine, JPSJ 25, 1100 (1968).
- (14) Carlson, Kaiser, Moser, Wahl, JCP 52, 4678 (1970).
- (15) Brewer, Wang, JCP 56, 4305 (1972).
- (16) Kalff, Alkemade, JCP 52, 2572 (1973).
- (17) Field, JCP 60, 2400 (1974).
- (18) Volnyets, Kovalenok, Sokolov, OS(Engl. Transl.) 36, 609
- (19) Ault, Andrews, JCP 62, 2320 (1975). | (1974).
- (20) Field, Capelle, Jones, JMS 54, 156 (1975).
- (21) Engelke, Sander, Zare, JCP 65, 1146 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{40}\text{Ca}^{32}\text{S}$		$\mu = 17.7617690$ $D_0^0 = 3.4_6 \text{ eV}^a$ Continuous absorption from 41860 cm^{-1} to higher wave numbers, observed and ascribed to CaS by (1), but questioned by (4).								JUL 1976
A $1\Sigma^+$	15220.79	409.04	Z 0.818	0.16666	0.00060 ₅	0.109	2.3864	A \leftarrow X, R	15194.44 Z	(4)
X $1\Sigma^+$	0	462.23	Z 1.78	0.17667	0.00083 ₇	0.102	2.3178			
$^{12}\text{C}^{(79)}\text{Br}$		$(\mu = 10.41616100)$ $D_0^0 \leq 4.11 \text{ eV}^a$								JUL 1976
A ₂ $2\Delta_{5/2}$	b	c		[0.4956]		[1.2]	} [1.815] ^e	A ₂ \leftarrow X ₂ , V 32753.10 Z (A ₂ \leftarrow X ₁) (33218.4) H (A ₁ \leftarrow X ₂) (32699.1) H A ₁ \leftarrow X ₁ , ^f 33163.5		(1)(2)*
A ₁ $2\Delta_{3/2}$		c		d						
X ₂ $2\Pi_{3/2}$	g	c		[0.4877]		[0.6]	} [1.823] ^h			
X ₁ $2\Pi_{1/2}$	0	c								
$^{12}\text{C}^{35}\text{Cl}$		$\mu = 8.93413850$ $D_0^0^a$								JUL 1976
A $2\Delta_r$	b	[848.1]	H	[0.7062 ₀]		[1.84]	[1.6346]	A \leftrightarrow X, V 35870.28 ^c Z 36003.92 ^c Z	(3)(4)(5)* (?)	
X $2\Pi_{3/2}$	d	[865.48]	Z	0.7009 ₉	0.00678	[1.89] ^e	1.6450			
X $2\Pi_{1/2}$	0	[866.72]	Z 6.2 H	0.6936 ^f	0.00672	[1.9] ^g	Theoretical work on low-lying valence states; see (9).			
$^{12}\text{C}^{(35)}\text{Cl}^+$										JUL 1976
A (1Π)	42350	922.5	H 21.5					A \rightarrow X, R 42220	H	(1)(2)
X (1Σ)	0	1175.0	H 5.0							

CaS: ^aThermochemical value (mass-spectrom.)(3), corrected for a ¹Σ ground state. Good agreement with (2).

(1) Mathur, PRS A 162, 83 (1937).

(2) Marquart, Berkowitz, JCP 39, 283 (1963).

(3) See ref. (9) of CaO.

(4) Blues, Barrow, TFS 65, 646 (1969).

CBr: ^aFrom the predissociation in $A_1^2\Delta_{3/2}(v=0)$. Study of flame reactions (3) suggests 2.8₆ eV.

^b $A_0 = + 28$.

^c $\Delta G''(\frac{1}{2}) - \Delta G'(\frac{1}{2}) = + 93.7 (F_1) \text{ and } + 82.8 (F_2)$.

^dBoth $v=0$ and $v=1$ of A_1 are predissociated.

^eFrom the "true" $B_0 = 0.4912$.

^fUndegraded diffuse band.

^g $A_0 = + 466$.

^hFrom the "true" $B_0 = 0.4872$.

(1) Simons, Yarwood, TFS 57, 2167 (1961).

(2) Dixon, Kroto, TFS 59, 1484 (1963).

(3) Miller, Palmer, JCP 40, 3701 (1964).

CCl_4 , CCl_4^+ :

^aStudy of flame reactions suggests $D_0^0 = 3.3_4$ eV (6).

^b $A_0 = + 7.04$; see (8).

^c $J'=3/2$ (average of F_1 and $\{F_2\}$) relative to $\{J''=0\}$.

^d $A_0 = + 134.92$.

^e $D_1 = 2.30 \times 10^{-6}$.

^f Λ -type doubling, $\Delta v = 0.0137(J+\frac{1}{2})$.

^g $D_1 = 2.0 \times 10^{-6}$.

(1) Barrow, Drummond, Walker, PPS A 67, 186 (1954).

(2) Kuzyakov, Tatevskii, NDVSK No. 2, 237 (1959).

(3) Gordon, King, CJP 39, 252 (1961).

(4) See ref. (1) of CBr.

(5) Verma, Mulliken, JMS 6, 419 (1961).

(6) See ref. (3) of CBr.

(7) Ovcharenko, Kuzyakov, Tatevskii, OS(Engl. Transl.) 19, 294 (1965).

(8) Merer, Travis, Watson, CJP 44, 447 (1966).

(9) Bialski, Grein, JMS 61, 321 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(II4, II2) Cd ₂		$(\mu = 56.447101_2) \quad D_0^0 = 0.08_0 \text{ eV}^a$ Large number of continua and diffuse bands. See (2), also (3)(4).								NOV 1974 A
(II4) Cd(79) Br		$(\mu = 46.618527_8) \quad 0.9 \text{ eV} \leq D_0^0 \leq 1.6 \text{ eV}^a$ <div><div><div>$C \left\{ \begin{array}{l} ({}^2\Pi_{3/2}) \quad 31463 \\ ({}^2\Pi_{1/2}) \quad (30300) \end{array} \right.$</div><div>$B ({}^2\Sigma)$</div><div>$X ({}^2\Sigma) \quad 0$</div></div><div><div>$253.8^b \text{ H} \quad 0.73$</div><div>$c$</div></div><div>Unclassified emission bands, $12300 - 30300 \text{ cm}^{-1}$.^d</div><div>$230.5^b \text{ H} \quad 0.50$</div></div>						<div>$C \leftrightarrow X, \quad V \left\{ \begin{array}{l} 31474 \quad \text{H} \\ 30310 \quad \text{H} \end{array} \right.$</div> <div>$B \rightarrow X, \quad R$</div>	<div>$(1)(5)(8)*$</div> <div>$(5)(7)(8)*$</div> <div>$(1)(3)(4)(5)(6)$</div>	NOV 1974
(II4) Cd ³⁵ Cl		$(\mu = 26.754959_0) \quad D_0^0 = 2.1_2 \text{ eV}^a$ <div><div><div>$E ({}^2\Sigma) \quad 45398.4$</div><div>$C ({}^2\Pi_r) \quad \left\{ \begin{array}{l} 32502 \\ 31485 \end{array} \right.$</div><div>$B ({}^2\Sigma)$</div><div>$X ({}^2\Sigma) \quad 0$</div></div><div><div>$264.0 \text{ H} \quad 7.5^b$</div><div>$399.0 \text{ H}^q \quad 1.5$</div><div>$0-0 \text{ sequence only.}^c$</div></div><div>Unclassified emission bands, $11500 - 30000 \text{ cm}^{-1}$.^d</div><div>$331.0 \text{ H} \quad 1.0$</div></div>						<div>$E \rightarrow X, \quad R \quad 45363.3 \quad \text{H}$</div> <div>$C \leftarrow X, \quad V \left\{ \begin{array}{l} 32536 \quad \text{H}^q \\ 31519 \quad \text{H}^q \end{array} \right.$</div> <div>$B \rightarrow X, \quad R$</div>	<div>$(5)* (7)*$</div> <div>$(1)(4)(6)(11)$</div> <div>$(2)(8)$</div>	NOV 1974
(II4) Cd ¹³³ Cs ?		$(\mu = 61.336453_4)$ Diffuse V shaded absorption bands at 18810 and 19120 cm^{-1} .								NOV 1974 (1)
(II4) Cd ¹⁹ F		$(\mu = 16.282568_9) \quad D_0^0 = (3.2) \text{ eV}^a$ "Bands" found in emission in the same region (1)(3) have been shown by (4) to be peculiar Cd lines. Narrow continuum at 35400 cm^{-1} , and unclassified bands in absorption at 35855 , 35877 , and 35897 cm^{-1} . <div><div><div>$E ({}^2\Sigma) \quad (34200)$</div><div>$X ({}^2\Sigma) \quad 0$</div></div><div><div>$(535) \text{ H}$</div><div>$(535) \text{ H}$</div></div></div>						<div>$E \leftarrow X,^b \quad R$</div>	<div>(2)</div> <div>(2)</div>	NOV 1974

- Cd_2 : ^aFrom temperature dependence of diffuse molecular absorption; average of the values obtained by (1) and (5).
 (1) Kuhn, Arrhenius, ZP 82, 716 (1933).
 (2) Finkelburg, "Kontinuierliche Spektren", Springer, Berlin (1938).
 (3) Garton, PPS A 64, 430 (1951).
 (4) Freedhoff, PPS 92, 505 (1967).
 (5) Bruner, Corbett, unpubl., quoted in DISSEN.
- CdBr : ^aNa D line chemiluminescence in Na/CdBr_2 flames [(2), revised].
^bAverage of constants given in (1) (em.) and (8) (abs.).
^cNo agreement between constants derived from the analysis of the emission spectrum by (7) ($w_e = 237.0$, $w_e x_e = 0.50$) and of the absorption spectrum by (8) ($w_e = 253.0$, $w_e x_e = 2.30$).
^dConstants suggested by (6) are $T_e = 24823$, $w_e = 105.4$, $w_e x_e = 1.70$.
 (1) Wieland, HPA 2, 46, 77 (1929).
 (2) Horn, Polanyi, Sattler, ZPC B 17, 220 (1932).
 (3) Oeser, ZP 95, 699 (1935).
 (4) Wieland, in "Contribution à l'Etude de la Structure Moléculaire", Vol. comm. Victor Henri, Ed. Desoer, Liège (1948), p. 229.
 (5) Ramasastry, IJP 23, 453 (1949).
 (6) Patel, Patel, IJP 41, 155 (1967).
 (7) Darji, IJPAP 8, 240 (1970).
 (8) Gosavi, Greig, Young, Strausz, JCP 54, 983 (1971).
- CdCl : ^aFrom temperature dependence of absorption spectrum (10).
 Na D line chemiluminescence in Na/CdCl_2 flames gives $1.3 \text{ eV} \leq D_0^0 \leq 2.1 \text{ eV}$ [(3), revised].
^bPredissociation suggested for $v > 1$.
^cRevised analysis (11).

CdCl (continued):

- ^dConstants suggested by (9) are $T_e = 26010$, $w_e = 153.5$, $w_e x_e = 3.75$.
 (1) Walter, Barratt, PRS A 122, 201 (1929).
 (2) See ref. (1) of CdBr .
 (3) See ref. (2) of CdBr .
 (4) See ref. (3) of CdBr .
 (5) Cornell, PR 54, 341 (1938).
 (6) Howell, PRS A 182, 95 (1943).
 (7) Ramasastry, IJP 21, 267 (1947).
 (8) See ref. (4) of CdBr .
 (9) Patel, Patel, IJPAP 4, 388 (1966).
 (10) See ref. (5) of Cd_2 .
 (11) Wieland, unpubl., quoted in DONNSPEC.

CdCs : (1) Barratt, TFS 25, 758 (1929).

CdF : ^aEstimated thermochemical value (5).

^bRather diffuse heads.

- (1) Pearse, Gaydon, PPS 50, 711 (1938).
 (2) Fowler, PR 62, 141 (1942).
 (3) See ref. (6) of CdCl .
 (4) Pearse, Feast, Nature 163, 686 (1949).
 (5) Besenbruch, Kana'an, Margrave, JPC 69, 3174 (1965).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(114)\text{Cd}^1\text{H}$		$(\mu = 0.99898612) \quad D_0^0 = 0.678 \text{ eV}^a$								NOV 1974 A
D								D \leftarrow X, V	44136 H	(9)
C	$2\Sigma^+$ (40202)	[1567]	H (50)	[6.00] ^b			[1.68]	C \leftarrow X, V	40314.9 Z	(7)* (9)*
B	$2\Sigma^+$ (24961)	(1000) ^c	(17)	[2.95] ^c			[2.39]	B \rightarrow X, R	24749.0 Z	(4)
A	$2\Pi \begin{Bmatrix} 3/2 \\ 1/2 \end{Bmatrix}$ 23116 ^d (22117)	1757.8 Z	38.6	6.143	0.205	2.9	1.657 ₄	A \rightarrow X, V	$\begin{Bmatrix} 23277.2 \\ 22276.5 \end{Bmatrix}$ Z	$\begin{Bmatrix} (1)* (2) (4) \\ (5) (6) \end{Bmatrix}$
X	$2\Sigma^+$ 0	[1337.1 ₄] Z	g	[5.323] ^h	i	[3.14] ^j	[1.780 ₅]	ESR sp. ^k		
$(114)\text{Cd}^2\text{H}$		$(\mu = 1.97910657)$								NOV 1974 A
D		[1056]	H					D \leftarrow X, V	44117 H	(9)
C	$2\Sigma^+$	[1149]	H (37)					C \leftarrow X, V	40260 H	(7)(9)*
A	$2\Pi \begin{Bmatrix} 3/2 \\ 1/2 \end{Bmatrix}$ ^l	[1209.7] Z		3.086	0.070	0.73	1.661 ₄	A \rightarrow X, V	$\begin{Bmatrix} 23236.4 \\ 22230.1 \end{Bmatrix}$ Z	$\begin{Bmatrix} (4) (5) \end{Bmatrix}$
X	$2\Sigma^+$ 0			[3.025]		[0.57]	[1.678 ₀]			
				[2.704] ^m	m	[0.76] ^m	[1.774 ₈]			
$(114)\text{Cd}^1\text{H}^+$		$D_0^0 = 2.1 \text{ eV}^a$								NOV 1974
A	$1\Sigma^+$ 42934.1	1252.0 Z	8.6	4.851	0.082	2.9 ^b	1.865 ₁	A \rightarrow X, R	42680.6 Z	(1)
X	$1\Sigma^+$ 0	1772.5 Z	35.40 ^c	6.071	0.190	2.9 ^{bd}	1.667 ₂			
$(114)\text{Cd}^2\text{H}^+$										NOV 1974
A	$1\Sigma^+$ 42930.6	887.2 Z	3.4 ₄	2.452	0.028	0.72 ^e	1.864	A \rightarrow X, R	42746.8 Z	(2)
X	$1\Sigma^+$ 0	1262.5 Z	19.0 ₁	3.075	0.068 ₂	0.48 ^f	1.664 ₃			
$(114)\text{Cd}^{(202)}\text{Hg}$		$(\mu = 72.830101_6)$ Continuous emission at 21300 cm^{-1} .								MAY 1976 (1)

Cd^1H , Cd^2H :

- ^aShort extrapolation of the ground state.
^bAll observed levels diffuse due to predissociation.
^cObserved up to $v=13$. More accurate constants will depend on the analysis of numerous perturbations by $\text{A } ^2\Pi$.
^d $A_0 = +1012.8$, $A_1 = +1016.2$.
^e Λ -type doubling $\Delta v_{fe}(v=0) = +0.62(J+\frac{1}{2}) - \dots$ (3).
^f $J'=\frac{1}{2}$ above $N''=0$. Svensson (4) uses a different definition.
^g $\Delta G(3/2, \dots, 9/2) = 1213.1_0, 1065.8_4, 881.1_0, 635.2$.
 Estimated zero point energy ≈ 708 .
^hSpin doubling $\Delta v_{12}(v=0) = +0.60(N+\frac{1}{2}) - \dots$ (3)(4)(8).
ⁱ γ decreases rapidly with increasing v .
^j $B_1, \dots, B_5 = 5.065, 4.758, 4.388, 3.893, 3.114$.
^k D_1, \dots, D_5 (10^{-4}cm^{-1}) = 3.38, 3.63, 5.00, 7.00, 16.00.
^lIn Ar matrix at 4 K (10).
^m $A_0 = +1012.4$.
ⁿ $B_1 = 2.536$, $D_1 = 1.78 \times 10^{-4}$. Spin doubling $\Delta v_{12}(v=0) \approx +0.31(N+\frac{1}{2}) - \dots$ (4)(8).
 (1) Bender, PR 36, 1543 (1930).
 (2) Watson, PR 36, 1134 (1930).
 (3) Mulliken, Christy, PR 38, 87 (1931).
 (4) Svensson, Dissertation (Stockholm, 1935).
 (5) Deile, ZP 106, 405 (1937).
 (6) Stenvinkel, Svensson, Olsson, AMAF A 26, No. 10 (1939).
 (7) Khan, PPS 80, 1264 (1962).
 (8) Veseth, JP B 3, 1677 (1970).
 (9) Breckenridge, Callear, TFS 67, 2009 (1971).
 (10) Knight, Weltner, JCP 55, 2061 (1971).

Cd^1H^+ , Cd^2H^+ :

- ^aValue given by Gaydon in DISSEN.
^bValues for H_v also reported in (1).
^c $w_e y_e = -0.371$.
^d $\beta_e = +0.1 \times 10^{-4}$.
^e $\beta_e = +0.08 \times 10^{-4}$.
^f $\beta_e = +0.12 \times 10^{-4}$.
 (1) Svensson, Tyrén, ZP 85, 257 (1933).
 (2) Zumstein, Gabel, McKay, PR 51, 238 (1937).

CdHg : (1) McGeoch, Fournier, Ewart, JP B 2, L121 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(114)Cd¹²⁷I										
		$(\mu = 60.026479_5) \quad 0.4 \text{ eV} \leq D_0^0 \leq 0.9 \text{ eV}^a$								NOV 1974
E ($^2\Sigma^+$)	(41912)	108.5 ^b H	1.0					E \rightarrow X, R (41877) ^b H		(1)(5)(6)
D ($^2\Pi_{3/2}$)	29531.7	196.8 ^c H	0.8 ₅					D \leftrightarrow X, V 29540.7 H		(1)(3)(6)* (7)(11)*
C ($^2\Pi_{1/2}$)	28230.5	188.2 ^d H	0.8 ₄					C \leftrightarrow X, (V) 28235.2 H		(5)(6)* (9)* (11)*
B ($^2\Sigma$)		Large number of emission bands from 15000 to 28000 cm^{-1} . ^e						B \rightarrow X, R		(1)(3)(4)(8) (10)
X ($^2\Sigma$)	0	178.7 ^f H	0.7 ₆							
(114)Cd⁽¹¹⁵⁾In										
		$(\mu = 57.200716_7)$ Diffuse bands in emission at 22160 and 24370 cm^{-1} , extending to longer wavelengths from the In lines at 4511 and 4102 \AA .								NOV 1974
(F)	e + 17549.3	76.2 ^a H						(F) \rightarrow (E), R 17535.2 ^a H		(2)
(E)	e	104.5 ^a H								(2)
D ($^2\Sigma$)	c + 17336.7 ^b	103.8 H	0.3					D \rightarrow C, ^c V 17354.9 H		(1)* (2)*
C ($^2\Sigma$)	c	67.3 H	0.1							
B ($^2\Pi$)	a + 18017.0	210.4 H						B \rightarrow A, ^c V 18038.6 H		(1)* (2)*
A ($^2\Sigma$)	a + 18008.8	212.2 H	0.15						18031.3 H	
	a	167.5 H	0.70							
(114)Cd⁽³⁹⁾K ?										
		$(\mu = 29.0323970)$ Diffuse V shaded absorption bands at 23850 and 23960 cm^{-1} .								NOV 1974 (1)
(114)Cd²³Na ?										
		$(\mu = 19.128878_9)$ Diffuse V shaded absorption bands at 24990 and 25160 cm^{-1} .								NOV 1974 (1)

CdI: ^aNa D line chemiluminescence in Na/CdI₂ flames [(2), revised].

^bVibrational numbering uncertain; compare (5) and (6).

^cAverage of constants obtained by (1) (emission) and (11) (absorption).

^dAverage of constants obtained by (9) (emission) and (11) (absorption).

^eIt was suggested by (10) that these bands form two separate systems and that for the system at shorter wavelengths $\nu_e = 23868.4$, $\omega_e' = 74.0$, $\omega_e'x_e' = 2.0$.

^fAverage of constants obtained by (1)(6)(9)(11).

(1) Wieland, HPA 2, 46, 77 (1929).

(2) Horn, Polanyi, Sattler, ZPC B 17, 220 (1932).

(3) Oeser, ZP 25, 699 (1935).

(4) Subbaraya, Rao, Rao, PIAS A 5, 372 (1937).

(5) Howell, PRS A 182, 95 (1943).

(6) Ramasastry, Rao, IJP 20, 100 (1946).

(7) Wieland, Herczog, HCA 29, 1702 (1946).

(8) Wieland, in "Contribution à l'Etude de la Structure Moléculaire", Vol. comm. Victor Henri, Ed. Desoer, Liège (1948), p. 229.

(9) Patel, Patel, Darji, IJPAP 5, 526 (1967).

(10) Patel, Patel, Darji, IJPAP 6, 342 (1968).

(11) Gosavi, Greig, Young, Strausz, JCP 54, 983 (1971).

CdIn: ^aFragments of a band system [system E of (2)] overlapping D→C.

^b $\nu_e = 17326.7$ in (2) seems erroneous.

^cWrongly attributed to HgIn by (1). More recently, it was suggested that the D-C system is, in fact, due to CdIn₂; see (3).

(1) Purbrick, PR 81, 89 (1951).

(2) Santaram, Winans, JMS 16, 309 (1965).

(3) Santaram, Vaidyan, Winans, JP B 4, 133 (1971).

CdK, CdNa:

(1) Barratt, TFS 25, 758 (1929).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
(114)Cd ¹⁶ O		($\mu = 14.0253946_g$)		$D_0^0 \leq 3.8_2 \text{ eV}^a$						DEC 1974
		Bands originally ascribed by (1) to CdO have later been shown by (2) to be due to Bi ₂ .								
(114)Cd ⁽⁸⁵⁾ Rb?		($\mu = 48.646891_4$)								DEC 1974
		Diffuse V shaded absorption bands at 22280 and 22600 cm ⁻¹ . Other unclassified bands in the region 22500 - 24000 cm ⁻¹ .								(1)
(114)Cd ⁽³²⁾ S		($\mu = 24.9646325$)		$D_0^0 \leq 2.0_4 \text{ eV}^a$						DEC 1974
		The assignment to CdS of two absorption continua with long wavelength limits at 31700 and 42500 cm ⁻¹ (1) appears doubtful in the light of mass-spectroscopic evidence (2)(3)(4).								
(114)Cd ⁽⁸⁰⁾ Se		($\mu = 46.965051_9$)		$D_0^0 \leq 1.9_9 \text{ eV}^a$						DEC 1974
		The assignment to CdSe of two absorption continua with long wavelength limits at 25500 and 43850 cm ⁻¹ (1) appears doubtful in the light of mass-spectroscopic evidence (2)(3).								
(114)Cd ⁽²⁰⁵⁾ Tl		($\mu = 73.217007_4$)								DEC 1974
		Continuous emission extending to longer wavelengths from the Tl line at 3775 Å. Intensity maxima at 26480, 25590, 24870 cm ⁻¹ .								(1)
		Broad "continuous" band in emission at 20520 cm ⁻¹ , accompanied by V shaded bands at 20929, 21018, 21109, 21199 cm ⁻¹ .								(1)
		Continuous emission extending to longer wavelengths from the Tl line at 5350 Å. Intensity maxima at 18690, 17790, 17460 cm ⁻¹ .								(1)
(140)Ce ₂		($\mu = 69.952742$)		$D_0^0 = 2.5 \text{ eV}^a$						DEC 1974

CdO: ^aThermochemical value (3).

- (1) Walter, Barratt, PRS A 122, 201 (1929).
- (2) Barratt, Bonar, PM 2, 519 (1930).
- (3) Brewer, Mastick, JCP 12, 834 (1951).

CdRb: (1) See ref. (1) of CdCs.

CdS: ^aThermochemical value (mass-spectrom.)(2)(3)(4).

- (1) Sen Gupta, PRS A 143, 438 (1933).
- (2) Colin, ICB 26, 1129 (1961).
- (3) Goldfinger, Jeunehomme, TFS 52, 2851 (1963).
- (4) Marquart, Berkowitz, JCP 32, 283 (1963).

CdSe: ^aThermochemical value (mass-spectrom.)(2).

- (1) Mathur, IJP 11, 177 (1937).
- (2) See ref. (3) of CdS.
- (3) Berkowitz, Chupka, JCP 45, 4289 (1966).

CdTe: (1) Santaram, Vaidyan, Winans, JP B 4, 133 (1971).

Ce₂: ^aAverage of several thermochemical values (mass-spectrom.)(1)(2)(3).

- (1) Balducci, De Maria, Guido, JCP 50, 5424 (1969).
- (2) Gingerich, CC (1969), 9.
- (3) Gingerich, Finkbeiner, JCP 54, 2621 (1971).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$(140)\text{Ce}^{(11)}\text{B}$		$(\mu = 10.2061713)$		$D_0^0 = 3.1_2 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{12}\text{C}$		$(\mu = 11.05204212)$		$D_0^0 = 4.7 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{(193)}\text{Ir}$		$(\mu = 81.102841)$		$D_0^0 = 6.0_2 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{14}\text{N}$		$(\mu = 12.7290315_8)$		$D_0^0 = 5.3_2 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{16}\text{O}$		$(\mu = 14.3538845_4)$		$D_0^0 = 8.1_8 \text{ eV}^a$						DEC 1974 A
Large number of bands in the region $11000 - 29000 \text{ cm}^{-1}(2)^*$. Tentative assignments by (4)(7), revising earlier assignments in (1)(2):										
D_1								$D_1 \leftrightarrow X_1$, R 21379.1	H^Q	(4)(7)
F_2		(772)		[0.35290]		[2.9_5]	[1.8242_6]	$F_2 \leftrightarrow X_2$, R 20834.21	Z	(4)(7)(1)
D_3								$D_3 \leftrightarrow X_3$, R 20516.1	H^Q	(7)(1)
C_1		(798)		[0.34984]		[2.6_9]	[1.8322_2]	$C_1 \leftrightarrow X_1$, R 20273.84	Z	(4)(7)
A_4								$A_4 \leftrightarrow X_4$, R 19871.7	H^Q	(7)
C_3								$C_3 \leftrightarrow X_3$, R 16356.9	H^R	(7)
G	1_{II}							$G \leftrightarrow Y_1$, R 15035.40	H^Q	(7)
B_2		(771)		[0.34705]		[2.8_1]	[1.8395_8]	$B_2 \leftrightarrow X_2$, R 13804.01	Z	(4)(7)(1)
A_2								$A_2 \leftrightarrow X_2$, R 12687.91	H^Q	(7)(1)
A_1		(749)		[0.34672]		[2.9_7]	[1.8404_5]	$A_1 \leftrightarrow X_1$, R 12595.75	Z	(4)(7)
A_3								$A_3 \leftrightarrow X_3$, V 12162.20	H^Q	(7)
Y_4	$(^3\Delta_3)^b$	(866)		[0.3506_5]		[2.3]	[1.8301]			
Y_3	$(^3\Delta_2)^b$	(509)		[0.3614]		[7.3]	[1.802_7]			
Y_2	$(^3\Delta_1)^b$	(844)		[0.35214]		[2.4_5]	[1.8262_3]			
Y_1	$1_{\Sigma}(+)^b$	(850)		[0.35790]		[2.5_4]	[1.8114_8]			

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(140) Ce^{16}O (continued)										
x_4 ($1\phi_3$) ^b	$x_2 + (2065)^c$	(818)		0.35710	0.00108	[2.71]	1.8135 ₀			
x_3 ($3\phi_4$) ^b		(932)		0.35377	0.00114	[2.03]	1.8220 ₂			
x_2 ($3\phi_3$) ^b	x_2	[822.76] (Z)	(3.09)	0.35779	0.00179	[2.69]	1.8117 ₅			
x_1 ($3\phi_2$) ^b		(862)		[0.35452]		[2.40]	[1.8200 ₉]			

CeB: ^aThermochemical value (mass-spectrom.)(1).
(1) Gingerich, JCP 53, 746 (1970).

CeC: ^aThermochemical value (mass-spectrom.)(1).
(1) Gingerich, JCP 50, 2255 (1969).

CeIr: ^aThermochemical value (mass-spectrom.)(1).
(1) Gingerich, JCS FT II 70, 471 (1974).

CeN: ^aThermochemical value (mass-spectrom.)(1).
(1) Gingerich, JCP 54, 3720 (1971).

CeO: ^aThermochemical value (mass-spectrom.)(3)(5)(6)(8).

^bThese states give rise to absorption bands at a temperature of 1900 °C (7). No details given for transitions from Y_2 , Y_3 , Y_4 .

^c $X_4(v=0)$ is at 2060.25 cm^{-1} above $X_2(v=0)$. All other separations are unknown [(7), no details].

- (1) Watson, PR 53, 639 (1938).
- (2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (3) Walsh, Dever, White, JPC 65, 1410 (1961).
- (4) Ames, Barrow, PPS 90, 869 (1967).
- (5) Ames, Walsh, White, JPC 71, 2707 (1967).
- (6) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).
- (7) Barrow, in DONNSPEC (1970).
- (8) Ackermann, Rauh, JCP 60, 2266 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(140)\text{Ce}^{(106)}\text{Pd}$		$(\mu = 60.276395)$		$D_0^0 = 3.3_0 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{(195)}\text{Pt}$		$(\mu = 81.454361)$		$D_0^0 = 5.7_1 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{103}\text{Rh}$		$(\mu = 59.293219)$		$D_0^0 = 5.6_5 \text{ eV}^a$						DEC 1974
$(140)\text{Ce}^{(32)}\text{S}$		$(\mu = 26.0247376)$		$D_0^0 = 5.8_6 \text{ eV}^a$						DEC 1974
$^{12}\text{C}^{19}\text{F}$		$\mu = 7.3545996_4$		$D_0^0 = 5.67 \text{ eV}^a$		$\text{I.P.} = 9.20 \text{ eV}^b$				AUG 1976
		Fragments of additional systems in the absorption spectrum above 50000 cm^{-1} .								(15)
C' $2\Sigma^+$				$[1.5327]^c$		$[3.3]$	$[1.223]$	C' \leftarrow X, V	53597.0	(15)
D 2Π	52272.5^d	1803.9	Z 13.0	1.7301	0.0193	6.5	1.1510	D \leftarrow X, V	52519.9^e	(15)
B $2\Delta_r$	49399.6^f	$[1153.3_4]$	Z 19.4 g H	1.320_6^h	0.022 $_8$	4.0	1.317 $_4$	B $^i \leftrightarrow$ X, R	49340.1^j Z	(1)* (2) (13)*
A $2\Sigma^+$	42692.9	1780.4 $_5$	Z 30.7 $_3$	1.7228^k	0.0189 l	$[6.80]^m$	1.1535	A $^n \leftrightarrow$ X, V	42924.17^o Z	(1)* (2)(3) (4)(5)(6) (15)
a $4\Sigma^-$	$(22000)^p$	$(1324)^p$	$(11)^p$	$(1.302)^p$	$(0.013)^p$					
X $2\Pi_r$	0^q	1308.1	Z 11.10 r	1.4172^s	0.0184 $_0^t$	6.5	1.2718	ESR sp. ($2\Pi_{3/2}$) u		(12)
CF^+, CF^-		Theoretical calculations (14).								AUG 1976

CePd: ^aThermochemical value (mass-spectrom.)(1).
 (1) Cocke, Gingerich, JPC 76, 2332 (1972).

CePt, CeRh: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, JCS FT II 70, 471 (1974).

CeS: ^aThermochemical value (mass-spectrom.)(1), revised (2).
 (1) See ref. (6) of CeO.
 (2) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

CF, CF⁺, CF⁻:

- ^aThermochemical value (mass-spectrom.)(17). From the pre-dissociation in A ²Σ⁺; D₀⁰ ≤ 5.74 eV.
^bPhotoionization (11) and electron impact (17) appearance potential measurements; supported by theoretical calculations (14).
^cLine width increases with N. Vibrational numbering uncertain.
^dA ≈ + 0.2 or + 6.5.
^eBy extrapolation from the 1-0, 2-0, and 3-0 bands; the 0-0 band was not observed.
^fA₀ = + 0.76. The alternative value, A₀ = + 4.48, leads to disagreement between observed and calculated relative line intensities (15).
^gw_ey_e = - 0.4.
^hStrong perturbations in v=2 (15).
ⁱRadiative lifetime τ(v'=0) = 18.8 ns (8)(10); f₀₀(B←X) = 0.022 (recalculated for a ²Δ upper state). See also (9).
^jJ'=3/2 (average of {F₁} and {F₂}) relative to J''=1/2 (average of F₁ and {F₂}). The band centres in (13) must all be reduced by 1.4 cm⁻¹ (15) owing to an error resulting from the incorrect application of the vacuum correction.
^kPredissociation above v=1, due to a curve crossing with the a ⁴Σ⁻ state at an internuclear distance smaller than r_e; see (15)(16).
^ly_e = - 0.0028 (B₀ and B₁ from (6), B₂ from (15)).
^mD₁ = 7.1₀ × 10⁻⁶ (6), D₂ = 9.0₀ × 10⁻⁶ (15).
ⁿRadiative lifetime τ(v'=1) = 19.0 ns (8)(10); f₀₀(A←X) ≈ 0.0027, f_{el} ≈ 0.026 (7)(10). See also (9).
^oN'=0 relative to J''=½ (average of F₁¹ and {F₂²}).

CF, CF⁺, CF⁻ (continued):

- ^pPreliminary results of theoretical calculations (15)(16).
^qA_v = + 77.12 - 0.655v + 0.0057v².
^rw_ey_e = + 0.093, w_ez_e = - 0.0011
^sΛ-type doubling; see (6).
^ty_e = + 0.00011.
^uμ_{el}(C⁻F⁺) = 0.65 D; polarity predicted by the theoretical work of (14) and (16).
 (1) Andrews, Barrow, Nature 165, 890 (1950); PPS A 64, 481 (1951).
 (2) Margrave, Wieland, JCP 21, 1552 (1953).
 (3) Mann, Broida, Squires, JCP 22, 348 (1954).
 (4) Kuzyakov, Tatevskii, OS 5, 699 (1958).
 (5) Thrush, Zwolenik, TFS 52, 582 (1963).
 (6) Porter, Mann, Acquista, JMS 16, 228 (1965).
 (7) Harrington, Modica, Libby, JCP 44, 3380 (1966); 45, 2720 (1966)(Erratum).
 (8) Hesser, Dressler, JCP 45, 3149 (1966).
 (9) Wentink, Isaacson, JCP 46, 603 (1967).
 (10) Hesser, JCP 48, 2518 (1968).
 (11) Walter, Lifshitz, Chupka, Berkowitz, JCP 51, 3531 (1969).
 (12) Carrington, Howard, MP 18, 225 (1970).
 (13) Carroll, Grennan, JP B 3, 865 (1970).
 (14) O'Hare, Wahl, JCP 55, 666 (1971).
 (15) W. P. White, Dissertation (Ohio State Univ., 1971), and C. W. Mathews, private communication.
 (16) Hall, Richards, MP 23, 331 (1972).
 (17) Hildenbrand, CPL 32, 523 (1975).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁴ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	ν ₀₀	
¹² C ¹ H		μ = 0.92974056 D ₀ ⁰ = 3.46 ₅ eV ^a I.P. = 10.64 eV ^b Several unassigned absorption bands ^c above 80000 cm ⁻¹ . Rydberg series joining on to G, ν = 85850 - R/(n - 0.09) ² ; n = 3,4,5,6								AUG 1976 A
G d	[74373]							G ← X,	72960	(26)*
F 2Σ ⁺	[65945]			[12.17] ^e			[1.221]	F ← X, R	64531.5 ^f Z	(26)*
E 2Π	[65625]			[12.6] ^g			[1.20]	E ← X, R	64211.7 ^f Z	(26)*
D 2Π _i	[60394] ^h			[13.7] ^g			[1.15]	D ← B, V	33282.8 ^f Z	(26)*
C 2Σ ⁺	31801.5	2840.2	Z 125.9 ₆ ⁱ	14.603 ^{jk}	0.7185 ^l	[15.55] ^m	1.1143	D ← X,	58981.0 ^f Z	(26)*
B 2Σ ⁻	(26044)	[1794.9] ^p	Z	[12.645] ^{qk}	r	[22.2] ^s	[1.1975]	C ⁿ ↔ X, ^o V _R	31778.1 ^f Z	(1)(3)(10)* (26)
A 2Δ	23189.8 ^u	2930.7	Z 96.65	14.934 ^{vk}	0.697	15.4 ^w	1.1019	B ^t ↔ X, ^o R	25698.2 ^f Z	(2)* (3) (10)* (26)*
a 4Σ ⁻	(5844)	(3145)	(72)	(15.4)	(0.55)		(1.08 ₅)	A ^x ↔ X, ^o V	23217.5 ^f Z	(3)(6)(10)* (12)*
X 2Π _r	0 ^z	2858.5	Z 63.0 ₂	14.457 ^{a'b'k}	0.534	14.5	1.1199		5985 ^y	(48)
								Λ doubling sp. ^{a'}		(39)
								Ab initio calculations;		ref. in (44)

C¹H: ^aFrom the predissociation in the B state (26) as modified by (41) and (49). Confirmed thermochemically by (13).

^bFrom Rydberg series (26). Theoretical photoionization cross section (36).

^cAccording to theoretical work (35) they represent the nf series.

^d3d complex consisting of 2Σ , 2Π , 2Δ .

^eSpin splitting constant $f_0 = +0.6_2$. Heterogeneous predissociation.

^fThe band origins refer to the zero points of the Hill-Van Vleck formulae for the ground and excited ($\Lambda \neq 0$) states. See also (11).

^gHomogeneous predissociation.

^h $\Lambda = -28.5$.

ⁱ $w_e y_e = +13.55$, $w_e z_e = -3.957$; from CD using isotope relations.

^jSpin splitting constant $\gamma \approx +0.05$ (26)(37). Predissociation, see n.

^kSlightly different sets of constants from the same data are

C¹H (continued):

given by (37) for X, A, B, C and (40) for X, A. Precise values for the rotational energy levels of X ²Π(v=0) in (15); tables of term values for levels of X, A, B, C in (37). $E + 0.0258(v+\frac{1}{2})^2 - 0.023(v+\frac{1}{2})^3$; see ¹.

^mD₁ = 16.7 x 10⁻⁴, D₂ = 20 x 10⁻⁴.

ⁿLifetime of C ²Σ⁺ anomalously small on account of predissociation (24)(26)(28)(38). According to (49) the lifetime in v=0 varies from 10 ns at N=1 to 25 ns at N=24 and is even shorter in v=1. The previous observation of different lifetimes for F₁ and F₂ levels is not confirmed. The lifetime for CD is more than twice that for CH (28) indicating that predissociation is weaker (26). Ab initio theory (46) gives a radiative lifetime τ(v=0) = 89 ns suggesting that the radiationless and the radiative transition probabilities are approximately in the ratio 8:1 (49). From absorption experiments (21) an f value of 0.006 was derived for the C-X transition.

^oWavenumber and wavelength tables and comparisons with the solar spectrum published by (7). ¹³CH lines for A-X measured by (23) and used to determine ¹³C/¹²C ratio in the sun. Franck-Condon factors (17)(33). The laboratory absorption spectrum was first observed by (5) in the acetylene combustion initiated by the flash photolysis of NO₂ in flames by (9); and more recently by (14)(19)(26).

^pVery shallow potential curve; ω_e ≈ 2251, ω_ex_e ≈ 230 (from CD). A small potential maximum has been established in this state (26); confirmed by theoretical calculations (32).

^qSpin splitting constant γ₀ = - 0.0285 (3), γ₁ = - 0.020 (26). Breaking off in emission above v'=0, N'=15 and v'=1, N'=6 and broadening in absorption at higher N' due to predissociation; see also ^t. Selective excitation of v'=1 in hydrogen flames and suppression of breaking off (4).

^rB₁ = 11.160.

^sD₁ = 32.8 x 10⁻⁴.

^tRadiative lifetime τ = 0.38 μs (20)(21)(28) corresponding to f ≈ 0.0029. (41) and (49) have measured lifetimes of individual rotational lines finding a regular increase from 0.32 to 0.38 μs from N'=2 to 14 (v'=0); sudden drop to 0.12 μs for N'=15 due to predissociation; see, however, (45). In v'=1 the lifetime is 0.40 μs until breaking off occurs between N'=6 and 7.

^uA = - 1.0₂ (26), see also (6)(37).

^vStark effect, μ_{ef}(v=0) = 0.89 D (42).

^wβ_e = +0.4 x 10⁻⁴.

^xLifetime τ(v=0) = 0.53₄ μs (49) corresponding to f = 0.0053; superseding earlier less precise values by (8)(20)(28)(31)(43). (34) from shock tube absorption measurements obtain f_e = 0.0019. A theoretical f₀₀ = 0.0068 is given in (46). The observation of a reduced lifetime in v=1 for N > 11 (49) suggests a weak predissociation probably caused by X ²Π.

^yT₀, from laser photoelectron spectrometry of CH⁻ (48). Theoretical calculations (32) give 5395 cm⁻¹. The vibrational and rotational constants given are theoretical values; see also (29).

^zA = + 27.95. Slightly higher values in (16) and (37).

^aΛ-type doubling, Δv ≈ 0.038 x N(N+1) - For the lowest J values more complicated formulae apply, see (15) and (16). The transition between the two Λ components of J=½ has been observed with its hyperfine structure in emission in interstellar clouds (39). The derived J=½ Λ-doublet separation is 3320.987 MHz, close to earlier predictions by (15)(30) and a subsequent theoretical calculation by (39a). Predicted Λ-doubling and hyperfine splittings for other J values in (47).

^bStark effect, μ_{ef} = 1.46 D (18).

(continued p. 143)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^2\text{H}$		$\mu = 1.72463610$		$D_0^0 = 3.50_0 \text{ eV}^a$		$\text{I.P.} = 10.64 \text{ eV}^b$				AUG 1976 A
G c								G \leftarrow X,	72955	(5)*
F $2\Sigma^+$	[65605]			[6.86] ^d			[1.194]	F \leftarrow X, R	64563.9 ^e Z	(5)*
D $2\Pi_i$	(59038) ^f	(2025)		[7.425]		[4.0]	[1.1474]	D \leftarrow B, V	33212.0 ^e Z	(5)*
C $2\Sigma^+$	31818.1	2081.3	Z 66.79 ^g	7.879 ^{hi}	0.283 ^j	[4.5] ^k	1.1138	C ⁱ \leftrightarrow X, ^l V _R	31801.3 ^e Z	(2)(5)
B $2\Sigma^-$	26043	1652.5 ^m	Z 123.8	7.104 ⁱ	0.341 ⁿ	[6.36] ^o	1.173 ₀	B ⁱ \leftrightarrow X, ^l R	25796.9 ^e Z	(1)(2)(5)
A 2Δ	23184.4	2203.3	Z 78.50	8.032	0.260	[4.5] ^p	1.1032	A \leftrightarrow X, ^l V	23225.1 ^e Z	(2)
X $2\Pi_r$	0 ^q	2099.7 ₅	Z 34.02	7.806 ^r	0.208	4.2	1.1190			

C^2H : ^aFrom the predissociation in B $2\Sigma^-$ of CD. The revised value of $D_0^0(\text{CH})$ would imply $D_0^0(\text{CD}) = 3.51_2 \text{ eV}$.

^bFrom I.P.(CH).

^cSee ^d of C^1H .

^dHeterogeneous predissociation.

^eSee ^f of C^1H .

^f $A = -27.7$.

^g $w_e y_e = +5.364$, $w_e z_e = -1.15$; these two constants are derived under the assumption that ΔG of X 2Π is linear in $v+\frac{1}{2}$.

^hSpin splitting constant $\gamma_0 = +0.06$ (5).

ⁱLifetime and predissociation see (4)(5)(6). For B $2\Sigma^-$, $v=0$, breaking off occurs above $N'=24$, for $v=1$ above $N'=16$. For C $2\Sigma^+$ the predissociation is much weaker for CD than for CH; see ⁿ of C^1H .

^j $+0.0075(v+\frac{1}{2})^2 - 0.005(v+\frac{1}{2})^3$.

^k $D_1, \dots, D_4 (10^{-4} \text{ cm}^{-1}) = 4.9, 5.2, 6.3, 9$.

^lFranck-Condon factors (3)(7).

^mThe B state is too shallow for these constants to have much physical meaning.

ⁿ $\gamma_e = -0.095$.

^o $D_1 = 7.2 \times 10^{-4}$, $D_2 = 13.9 \times 10^{-4}$.

^p $D_1 = 4.7 \times 10^{-4}$.

^q $A = +27.95$.

^r Λ -type doubling, $\Delta v \approx 0.009 \times N(N+1)$ for higher N values. The splitting for $J=\frac{1}{2}$ is predicted (8) to be 1241 MHz.

(1) See ref. (2) of C^1H .

(2) Gerö, ZP 117, 709 (1941).

(3) See ref. (17) of C^1H .

(4) See ref. (24) of C^1H .

(5) See ref. (26) of C^1H .

(6) See ref. (28) of C^1H .

(7) See ref. (33) of C^1H .

(8) Hammersley, Richards, ApJ 194, L61 (1974).

C¹H (continued):

- (1) Heimer, ZP 78, 771 (1932).
- (2) Shidei, JJP 11, 23 (1936).
- (3) Gerö, ZP 118, 27 (1941).
- (4) Durie, PPS A 65, 125 (1952).
- (5) Norrish, Porter, Thrush, PRS A 216, 165 (1953).
- (6) Kiess, Broida, ApJ 123, 166 (1956).
- (7) Moore, Broida, JRNBS A 63, 19 (1959).
- (8) Bennett, Dalby, JCP 32, 1716 (1960).
- (9) Gaydon, Spokes, van Suchtelen, PRS A 256, 323 (1960).
- (10) Bass, Broida, NBSM No. 24 (1961).
- (11) Garstang, PPS 82, 545 (1963).
- (12) Pearse, Gaydon, IDSPEC (1963).
- (13) Brewer, Kester, JCP 40, 812 (1964).
- (14) Bleekrode, Nieuwpoort, JCP 43, 3680 (1965).
- (15) Douglas, Elliot, CJP 43, 496 (1965).
- (16) Goss, ApJ 145, 707 (1966).
- (17) Halmann, Laulicht, ApJ(Suppl.) 12, 307 (1966).
- (18) Phelps, Dalby, PRL 16, 3 (1966).
- (19) Bleekrode, Thesis (Amsterdam, 1966);
PRR(Suppl.) No. 7 (1967).
- (20) Fink, Welge, JCP 46, 4315 (1967).
- (21) Linevsky, JCP 47, 3485 (1967).
- (22) Pathak, Singh, IJPAP 5, 139 (1967).
- (23) Richter, Tonner, ZA 67, 155 (1967).
- (24) Hesser, Lutz, PRL 20, 363 (1968).
- (25) Sharma, Singh, Pathak, IJPAP 6, 443 (1968).
- (26) Herzberg, Johns, ApJ 158, 399 (1969).

C¹H (continued):

- (27) Le Calvé, Bourène, Schmidt, Clerc, JP(Paris) 30, 807 (1969).
- (28) Hesser, Lutz, ApJ 159, 703 (1970).
- (29) Liu, Verhaegen, JCP 53, 735 (1970).
- (30) Baird, Bredohl, ApJ 169, L83 (1971).
- (31) Smith, JCP 54, 1384 (1971).
- (32) Lie, Hinze, Liu, JCP 57, 625 (1972); 59, 1872, 1887 (1973).
- (33) Liszt, Smith, JQSRT 12, 947 (1972).
- (34) Kuz'menko, Kuzyakov, Kuznetsova, Kudryumova, Chuev, HT(USSR) 2, 823 (1972).
- (35) Walker, Kelly, JCP 57, 936 (1972).
- (36) Walker, Kelly, CPL 16, 511 (1972).
- (37) Botterud, Lofthus, Veseth, PS 8, 218 (1973).
- (38) Elander, Smith, ApJ 184, 663 (1973).
- (39) Rydbeck, Elldér, Irvine, Nature 246, 466 (1973); Rydbeck, Elldér, Irvine, Sume, Hjalmarson, AA 34, 479 (1974).
- (39a) Hammersley, Richards, Nature 251, 597 (1974).
- (40) Krupp, ApJ 189, 389 (1974).
- (41) Brooks, Smith, ApJ 194, 513 (1974).
- (42) Scarl, Dalby, CJP 52, 1429 (1974).
- (43) Jørgensen, Sørensen, JCP 62, 2550 (1975).
- (44) Meyer, Rosmus, JCP 63, 2356 (1975).
- (45) Anderson, Peacher, Wilcox, JCP 63, 5287 (1975).
- (46) Hinze, Lie, Liu, ApJ 196, 621 (1975).
- (47) Levy, Hinze, ApJ 200, 236 (1975).
- (48) Kasdan, Herbst, Lineberger, CPL 31, 78 (1975).
- (49) Brzozowski, Bunker, Elander, Erman, ApJ 207, 414 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^1\text{H}^+$										
$D_0^0 = 4.08_5 \text{ eV}^a$										
B 1Δ	(52534)	2075.5	Z 76.3	11.937	0.620	13 ^b	1.2325	$B^c \rightarrow A$, V	28537.9 Z	(5)(7)*
b $3\Sigma^-$	(38200)	[1939]		11.705 ^d	0.538	13.5	1.2446	$b^e \rightarrow a$, R	28580	(5)(7)*
A 1Π	(24111)	1865.35	Z 115.85 ^f	11.898 ₈ ^{ghi}	0.9414 ^j	20	1.2344	$A^k \leftrightarrow X$, ^l R	23596.9 ₄ Z	(1)* (2)*
a 3Π	(9200) ^m	(2814)		14.048 ⁱ	0.603	14	1.1361			
X $1\Sigma^+$	0	[2739.70]	Z (64) ⁿ	14.177 ₆ ⁱ	0.4917	14	1.1309			
$^{12}\text{C}^2\text{H}^+$										
$D_0^0 = 4.13 \text{ eV}^a$										
A 1Π	(24138)	[1248.5]	(Z)					$A^b \rightarrow X$, R	23747.6 (Z)	(1)
X $1\Sigma^+$	0	[2029.3]	(Z)							
$^{12}\text{C}^1\text{H}^-$										
$D_0^0 = 3.43_5 \text{ eV}^a$ I.P. = 1.238 eV ^b										
a 1Δ	(6828)	(3000)					(1.10) ^c		6815 ^d	(2)
X $3\Sigma^-$	0	(3025)					(1.08 ₉) ^c			
$^{12}\text{C}^{127}\text{I}$										
$\mu = 10.96331634$ a										
AUG 1976										

$C^1\text{H}^+$: $a D_0^0(C^1\text{H}) + \text{I.P.}(C) - \text{I.P.}(C^1\text{H})$.

$b \beta_e = 3 \times 10^{-4}$.

^cLifetime 0.22 μs [average of (8)(19)(21)].

^dMass-spectrometric observations suggest a predis-sociation of this state for $v > 1$ into the $3\Sigma^+$ state arising from $C^+(^2\text{P}) + \text{H}(^2\text{S})$; see (10)(17).

^eLifetime 0.48 μs (19).

^f $w_{ey} = +2.64$. These constants do not fit higher vibrational levels.

$C^1\text{H}^+$ (continued):

^e Λ -type doubling, $\Delta v_{ef}(v=0) = +0.0398 \text{ J}(J+1)$. The splitting decreases with increasing v .

^hTables of term values, and somewhat different constants based on the same data, are given by (14).

ⁱTheoretical potential functions for all states arising from $C^+(^2\text{P}) + \text{H}(^2\text{S})$ are given by (11). A 1Π RKR curve

^j $y_e = -0.0019$. See ^f. | in (4).

C^1H^+ (continued):

^kThere is considerable disagreement between lifetime measurements by different authors:

	v =	0	1	2	3	4	
Ref. (19): $\tau = 408$			495	530	465	525	ns,
Ref. (21): $\tau = 250$			270	290			ns.

Earlier determinations (9)(13) gave much lower values probably because of overlapping N_2 bands. Following are the averaged f values recommended by (21): $f_{00} = 0.013_6$, $f_{10} = 0.009_1$, $f_{20} = 0.003_6$. The theoretical values (18) are $f_{00} = 0.00645$, $f_{10} = 0.00431$, $f_{20} = 0.00173$.

^lOccurs in interstellar absorption (1)(6)(16). Franck-Condon factors (from ab initio potential energy curves) in (15); see also (3)(22).

^mFrom a theoretical calculation (11). $A \approx 23$ (7).

ⁿAverage of a theoretical value (20) and several estimates based on experimental results.

- (1) Douglas, Herzberg, CJR A 20, 71 (1942).
- (2) Douglas, Morton, ApJ 131, 1 (1960).
- (3) Nicholls, Fraser, Jarman, McEachran, ApJ 131, 399 (1960).
- (4) Read, Vanderslice, Jenč, JCP 37, 205 (1962).
- (5) Carré, Dufay, CR B 266, 1367 (1968).
- (6) Herbig, ZA 68, 243 (1968).
- (7) Carré, Physica 41, 63 (1969).
- (8) See ref. (28) of C^1H .
- (9) See ref. (31) of C^1H .
- (10) Lorquet, Lorquet, Wankenne, Momigny, Lefebvre-Brion, JCP 55, 4053 (1971).
- (11) Green, Bagus, Liu, McLean, Yoshimine, PR A 5, 1614 (1972).
- (12) See ref. (33) of C^1H .
- (13) Anderson, Wilcox, Sutherland, NIM 110, 167 (1973).

C^1H^+ (continued):

(14) See ref. (37) of C^1H .

(15) Green, Hornstein, Bender, ApJ 172, 671 (1973).

(16) Hobbs, ApJ 181, 79 (1973).

(17) Newton, Sciamanna, JCP 58, 1292 (1973).

(18) Yoshimine, Green, Thaddeus, ApJ 183, 899 (1973).

(19) Brzozowski, Elander, Erman, Lyyra, ApJ 193, 741 (1974).

(20) Banyard, Taylor, JP B 8, L137 (1975).

(21) Brooks, Smith, ApJ 196, 307 (1975).

(22) Rao, Murty, Rao, Rao, PL A 54, 177 (1975).

C^2H^+ : ^aFrom the value for C^1H^+ .

^bLifetime $\tau(v=0) = 64$ ns (2); $f_{00} = 0.06_2$. This value seems doubtful when compared with more recent results for C^1H^+ ; see ^k of C^1H^+ .

(1) Cisak, Rytel, APP A 39, 627 (1971).

(2) See ref. (31) of C^1H .

C^1H^- : ^aFrom $D_0^0(C^1H)$ and the electron affinities of C^1H [= I.P.(CH^-)] and C (1.268 eV).

^bFrom laser photoelectron spectrometry of CH^- (2). A theoretical value by (1) is $1.6_1 \pm 0.3$ eV.

^cIndirectly from a Franck-Condon analysis.

^d T_0 , from the photodetachment spectrum of CH^- .

(1) Cade, PPS 91, 842 (1967).

(2) See ref. (48) of C^1H .

CI: ^aStudy of flame reactions (1) suggests $D_0^0 = 2.1_7$ eV.

(1) Miller, Palmer, JCP 40, 3701 (1964).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	v ₀₀	
³⁵ Cl ₂		μ = 17.4844268 ₀ D ₀ ⁰ = 2.47936 ₇ eV ^a I.P. = 11.50 eV ^b Rydberg series joining on to P: v(1-0) = 93200 - R/(n - 0.54) ² , n = 3...7; fragmentary vibrational structure. Fragments of additional band systems in absorption at v > 65000 cm ⁻¹ . Emission continua in the ultraviolet with maxima at 32640, 33810, 34700, 35450, 36220, 36820, 38970, 41140, 42500, 43710, 45500, 46610, 47670; 50060, 51850, 53890 cm ⁻¹ . ^c								SEP 1976 A (9) (8)(9) (3)
P	(74405)	(621)	(3)	[0.184 ₀] ^d [0.119 ₃] ^d				P← X,	74436	(8)(9)
O								O→ X,	R 74018.5 ^d Z	(41)*
N								N→ X,	R 73363.3 ^d Z	(41)*
M	(72853)	(636)	(4)					M← X,	72891	(8)
K	(64024)	(460)						K→ X, ^e	63975	(5)
J	(61638)	(520)	(3)					J← X,	61618	(8)
I	61438	262.3	H 0.812					I→ B,	V 43632 H	(7)
H	(59432)	(510)						H← X,	59408	(8)
G	(58629)	(208)						G→ X, ^e R	58454	(5)
F	(58263)	(442)						F← X,	58205	(8)
E	57953	249.75	H 0.875					E↔ B,	R 40140.0 H	(6)(13)* (34)
D	(53568)	(440)	(1.5)					D← X,	53508	(8)
		Continuous absorption above ~52600 cm ⁻¹ at high pressure.								(1)(8)
C	1Π _u	Continuous absorption with maximum at 30500 cm ⁻¹ .						C↔ X, ^f		(2)(4)(15) (18)(19)
B	3Π ₀ ⁺ +u	17809	259.5 ^g	H 5.3 ^h	0.1625 ₆ ⁱ	0.0021 ₂ ^j	2.365 ^k	2.435 ₄	B ^l ↔ X, ^m R 17658 ^g	H (14)* (16)* (23)*

- Cl_2 : ^aFrom the convergence limit in $\text{B } ^3\Pi_0^+$ (see ^h). From the same limit (36) gives $D_0^0 = 19997.14 \text{ cm}^{-1}$ or 2.47934_9 eV presumably by using a different value for the $^2P_{1/2} - ^2P_{3/2}$ energy difference in Cl I . Here we used 882.36 cm^{-1} from (22).
- ^bFrom the photoelectron spectrum; average of (25) and (29). Photoionization (12), in agreement with the Rydberg series, yields 11.48 eV .
- ^cThey have been interpreted (3) as being due to transitions from stable excited states at 58000 (possibly F), 67700 and 75000 cm^{-1} to the repulsive states arising from $^2P + ^2P$. The upper states at 67700 and 75000 cm^{-1} are considered to be 1_g states and, therefore, are not observed in absorption from the ground state.
- ^dUpper levels of four extensive resonance series (10)(41). The v' values are uncertain. The resonance fluorescence spectrum is excited by the Cl I lines at 73983 and 73344 cm^{-1} in a discharge through Cl_2 and involves transitions to ground state levels with $v'' \leq 59$. The ground state dissociation energy derived from these resonance series (41) agrees now very well with the more accurate value from the B-X system.
- ^eThese systems [called J-X and H-X by (5)] have not been observed in absorption. For this reason (8) suggest that they may actually be due to Cl_2^+ .
- ^fThe angular distribution of photo-fragments confirms the assignment of the upper state of the continuum to $1\Pi_u$ (21); see also (35) and (40). The B-X transition, however, contributes to the weak low-frequency region of the continuum; for a discussion of quantitative data see (36a).

- ^gSince high resolution data (14)(23) are available only for $v \geq 5$ the constants given here are from the low resolution emission work of (16) (band heads); they are valid only for $0 \leq v \leq 6$. For $6 < v < 22$, (11) give $\omega_e = 259.57$, $\omega_e x_e = 4.75_3$, $\omega_e y_e = -0.067_7$, $\omega_e z_e = +0.00212$. The band origin of the $6-0$ band is at 18993.79 cm^{-1} .
- ^hConvergence limit $20879.64 \pm 0.14 \text{ cm}^{-1}$ (36)(38). See (28) (30)(32)(37)(38) and the review in (36) for relation of high vibrational levels to long-range internuclear potential.
- ⁱThese constants are based on bands with $5 \leq v' \leq 13$ (23). B_v values up to $v = 31$ have been determined (14)(23).
- ^j $r_e = -0.00009_1$.
- ^k $+0.225 \times 10^{-7}(v+\frac{1}{2}) + 0.015 \times 10^{-7}(v+\frac{1}{2})^2$. See ⁱ.
- ^lEstimated radiative lifetimes in (36a).
- ^mFranck-Condon factors from RKR potentials (26). For a discussion of the repulsive part of the potential see (35).

(continued p. 148)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{35}\text{Cl}_2$ (continued)										
A ($^3\Pi_{1u}$)	(17440)	(265)	H (5)					$A^l \rightarrow X, n$		(36a)
A' ($^3\Pi_{2u}$)	(17160) ^o	(280) ^p						$A' \rightarrow X, q$		(42)
X $1\Sigma_g^+$	0	559.7 ₂ ^{rs}	Z 2.67 ₅ ^t	0.2439 ₉ ^r	0.0014 ₉ ^u	1.86	1.987 ₉	Pressure induced IR absorption at 549 cm^{-1} Raman sp.		(20) (24)(27)(31) (33)(43)

Cl_2 (continued):

ⁿTwo weak progressions, not belonging to B-X and tentatively assigned as 1-v" and 2-v" with v" = 8, 9, ..., were observed in the chlorine atom recombination spectrum and in the spectrum of the nitrogen trichloride decomposition flame; see references in (36a).

^oNot observed in the gas phase (see ^q); in an Ar matrix this new state is located 650 cm^{-1} below the B $^3\Pi_{0+u}$ state.

^pEstimated from isotope shifts.

^qLong-lived (~ 76 ms in Ar) emission in rare gas matrices from v=0 of a new low-lying state following excitation into the B or C state; see (42).

^rThese constants are based on the lowest six vibrational levels (23). The following Dunham coefficients have been derived by (41) from a detailed analysis at high resolution of the resonance series excited by the Cl I lines at 1351.7 and 1363.5 \AA ; they represent all levels up to v=40:

$$Y_{10} = 559.7507$$

$$Y_{20} = -2.694271$$

$$Y_{30} = -3.32527 \times 10^{-3}$$

$$Y_{40} = -2.27337 \times 10^{-4}$$

$$Y_{50} = 3.92041 \times 10^{-6}$$

$$Y_{60} = -6.02984 \times 10^{-8}$$

$$Y_{00} = -0.0351$$

$$Y_{01} = 0.244153$$

$$Y_{11} = -0.0015163$$

$$Y_{21} = -3.9078 \times 10^{-6}$$

$$Y_{31} = 7.0811 \times 10^{-8}$$

$$Y_{41} = -5.5875 \times 10^{-9}$$

$$Y_{02} = -1.9195 \times 10^{-7}$$

$$Y_{32} = -3.1678 \times 10^{-12}$$

The same authors give, in addition, $G(v)$ and B_v values up to v=59 and have determined an accurate RKR potential function. The long-range portion agrees very well with that predicted from theory.

^s550.8 in liquid Cl_2 (33); 554.6 in solid argon (39)(42).

$$^t w_e y_e = -0.0067.$$

$$^u r_e = -0.0000017.$$

Cl₂ (continued):

- (1) Cordes, Sponer, ZP 63, 334 (1930).
- (2) Gibson, Bayliss, PR 44, 188 (1933); Gibson, Rice, Bayliss, PR 44, 193 (1933).
- (3) Asundi, Venkateswarlu, IJP 21, 101 (1947); Venkateswarlu, PIAS A 26, 22 (1947).
- (4) Sulzer, Wieland, HPA 25, 653 (1952).
- (5) Haranath, Rao, JMS 2, 428 (1958).
- (6) Venkateswarlu, Khanna, PIAS A 42, 117 (1959).
- (7) Khanna, PIAS A 42, 293 (1959).
- (8) Lee, Walsh, TFS 55, 1281 (1959).
- (9) Iczkowski, Margrave, Green, JCP 33, 1261 (1960).
- (10) Rao, Venkateswarlu, JMS 9, 173 (1962).
- (11) Richards, Barrow, PCS (1962), 297.
- (12) Watanabe, Nakayama, Mottl, JQSRT 2, 369 (1962).
- (13) Briggs, Norrish, PRS A 276, 51 (1963).
- (14) Douglas, Møller, Stoicheff, CJP 41, 1174 (1963).
- (15) Jacobs, Giedt, JQSRT 5, 457 (1965).
- (16) Clyne, Coxon, PRS A 298, 424 (1967).
- (17) Todd, Richards, Byrne, TFS 63, 2081 (1967).
- (18) Clyne, Stedman, TFS 64, 1816 (1968).
- (19) Palmer, Carabetta, JCP 49, 2466 (1968).
- (20) Winkel, Hunt, Clouter, JCP 50, 1298 (1969).
- (21) Busch, Mahoney, Morse, Wilson, JCP 51, 449 (1969).
- (22) Radziemski, Kaufman, JOSA 59, 424 (1969).
- (23) Clyne, Coxon, JMS 33, 381 (1970).
- (24) Holzer, Murphy, Bernstein, JCP 52, 399 (1970).
- (25) Cornford, Frost, McDowell, Ragle, Stenhouse, JCP 54, 2651 (1971).
- (26) Coxon, JQSRT 11, 443, 1355 (1971).
- (27) Hochenbleicher, Schrötter, AS 25, 360 (1971).
- (28) Le Roy, Bernstein, JMS 37, 109 (1971).
- (29) Potts, Price, TFS 67, 1242 (1971).
- (30) Goscinski, MP 24, 655 (1972).
- (31) Hendra, Vear, SA A 28, 1949 (1972).
- (32) Le Roy, CJP 50, 953 (1972).
- (33) Wallart, CJS 17, 128 (1972).
- (34) Wieland, Tellinghuisen, Nobs, JMS 41, 69 (1972).
- (35) Child, Bernstein, JCP 59, 5916 (1973).
- (36) Le Roy, in "Molecular Spectroscopy", Vol. 1, p. 113. The Chemical Society (1973).
- (36a) Coxon, in "Molecular Spectroscopy", Vol. 1, p. 177. The Chemical Society (1973).
- (37) Yee, Stone, MP 26, 1169 (1973).
- (38) Le Roy, CJP 52, 246 (1974).
- (39) Ault, Howard, Andrews, JMS 55, 217 (1975).
- (40) Brith, Rowe, Schnepp, Stephens, CP 2, 57 (1975).
- (41) Douglas, Hoy, CJP 53, 1965 (1975).
- (42) Bondybey, Fletcher, JCP 64, 3615 (1976).
- (43) Edwards, Good, Long, JCS FT II 72, 927 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{35}\text{Cl}_2^+$										
$B(2\Sigma_g^+)$ (34400) ^b		$\mu = 17.4842896_5$		$D_0^0 = 3.95 \text{ eV}^a$						SEP 1976
$A_2(2\Pi_{\frac{1}{2}}u)$		c		$[0.1778]^d$		c		$[2.329]^d$		$A_2 \rightarrow X_2, R \quad 22746.9_6^d Z \quad (4)^*$
$A_1(2\Pi_{\frac{3}{2}}u)$		c		$[0.1788]^d$		c		$[2.322]^d$		$A_1 \rightarrow X_1, R \quad 22199.5_4^d Z \quad (4)^*$
$X_2(2\Pi_{\frac{1}{2}}g)$ 645 ^b		644.77	Z	2.988	0.2697	0.00167		1.890 ₇		
$X_1(2\Pi_{\frac{3}{2}}g)$ 0		645.61	Z	3.015 ^e	0.2695 ₀	0.00164	1.8	1.8915		
$(^{35})\text{Cl}_2^-$										
$(2\Pi_g)$ [79400]		$(\mu = 17.4845639_4)$		$D_0^0 = 1.26 \text{ eV}^a$		I.P. = 2.39 eV ^b				SEP 1976 A
$X(2\Sigma_u^+)$ [0]		650 ^c								(6)
For computed ground state characteristics see (3).										
$^{35}\text{Cl}^{19}\text{F}$										
$B(3\Pi_0^+)$ 18826.4		$\mu = 12.3102869$		$D_0^0 = 2.617_3 \text{ eV}^a$		I.P. = 12.66 eV ^b				SEP 1976 A
For binding energies of F(1s) and Cl(2s) core electrons in ClF see (14).										
$X(1\Sigma^+)$ 0		363.1	Z	8.6 ₄ ^c	0.3319 ^d	0.0047 ^e	(10)	2.031	$B \leftarrow X, R \quad 18614.3_3^f Z$	(2)(5)
		786.15 ^g	Z	6.16 ₁ ^g	0.516478 ₈	0.004357 ₇	8.7 ₇	1.628313	Infrared sp., Raman sp. (liquid), microwave and mol. h beam el. reson. sp..	(3) (1) (9)(15)
$(^{35})\text{Cl}^{19}\text{F}^+$										
$B(2\Sigma^+)$ (41500) ^j		$D_0^0 = 2.93 \text{ eV}^i$								SEP 1976
$A(2\Pi)$ (29500) ^j										(7)(10) (7)(10)
$X\begin{cases} 2\Pi_{\frac{1}{2}} \\ 2\Pi_{\frac{3}{2}} \end{cases}$ 630 ^j 0		870 ^k								(7)(10)

Cl_2^+ : ^aFrom $D_0^0(Cl_2)$, I.P.(Cl_2), and I.P.(Cl).

^bFrom the photoelectron spectrum (5)(6).

^cSeveral higher vibrational levels have been observed and analyzed (4) but they do not form regular progressions. The vibrational constants quoted in (1a) from (1) just as the later values of (2) must be considered as erroneous (4). The partial rotational analysis of (3) agrees essentially with the more extensive one of (4).

^dLowest observed vibrational level, not necessarily $v=0$;

^e $\omega_e \nu_e = + 0.007$. | see ^c.

(1) Elliott, Cameron, PRS A 158, 681 (1937); 164, 531,

(1a) Herzberg, MOLSPEC 1 (1950). | (1938).

(2) Haranath, Rao, IJP 32, 401 (1958).

(3) Rao, Rao, CJP 36, 1557 (1958).

(4) Huberman, JMS 20, 29 (1966).

(5) See ref. (25) of Cl_2 .

(6) See ref. (29) of Cl_2 .

Cl_2^- : ^aFrom $D_0^0(Cl_2)$ and the electron affinities of Cl_2 and Cl (3.613 eV).

^bFrom endoergic charge transfer (2)(4)(5)(7); slightly higher value (2.5₂ eV) from dissociative electron attachment (1).

^cSingle progression of resonances in the scattering of electrons by Cl_2 indicating the existence of a doubly excited (preionizing) state of Cl_2^- with the $X^2\Pi_g$ state of Cl_2^+ as "grandparent" (6).

(1) DeCorpo, Franklin, JCP 54, 1885 (1971).

(2) Chupka, Berkowitz, Gutman, JCP 55, 2724 (1971).

(3) Gilbert, Wahl, JCP 55, 5247 (1971).

(4) Baede, Physica 59, 541 (1972).

(5) Hughes, Lifshitz, Tiernan, JCP 52, 3162 (1973).

(6) Spence, PR A 10, 1045 (1974).

(7) Tang, Leffert, Rothe, Reck, JCP 62, 132 (1975).

ClF , ClF^+ ;

^aOf the two possible values derived from the convergence of the B-X system thermochemical data (16) strongly favour the higher value given here. But (17) considers the lower value (2.558₁ eV) equally likely; see also (6).

^bFrom the photoelectron spectrum (7)(10); in good agreement with photoionization [12.65 eV (6)] and electron impact [12.7 eV (4)] appearance potentials.

^c $\omega_e \nu_e = - 0.12_4$. The vibrational and rotational constants have been recalculated from data in (5) for $3 \leq v \leq 8$.

Lower levels are not observed, higher levels are affected by a perturbation. See also (13). Convergence of $v'-0$ absorption progression at 21514 cm^{-1} .

^dPredissociation (diffuseness) of 11-0, 12-0, 13-0 bands at 21254 - 21399 cm^{-1} . See ^c.

^e $\gamma_e = - 0.00047_7$; see ^c.

^fExtrapolated from the 3-0 band.

^gRecalculated by (17) from the infrared data of (3). ν_0 of the fundamental, 773.83 cm^{-1} , agrees rather poorly with $\Delta G(\frac{1}{2}) = 773.46$ from the electronic absorption spectrum (5).

^h $\mu_{el}(v=0) = 0.8881$ D (9); the sign of the dipole moment is + ClF^- (11)(14)(18), see however (8)(12). $eqQ(Cl)$ and other hyperfine structure constants in (9)(15). Zeeman effect (8), $g_J = - 0.1089 \mu_N$.

ⁱFrom $D_0^0(ClF)$, I.P.(ClF), and I.P.(Cl).

^jFrom photoelectron spectra (7)(10).

^kFrom (10); (7) give 912 ± 30 cm^{-1} .

(1) Jones, Parkinson, Burke, JCP 18, 235 (1950).

(2) Schumacher, Schmitz, Brodersen, AAQA 38, 98 (1950).

(3) Nielsen, Jones, JCP 19, 1117 (1951).

(4) Irsa, Friedman, JINC 6, 77 (1958).

(5) Stricker, Krauss, ZN 23 a, 1116 (1968).

(6) Dibeler, Walker, McCulloh, JCP 53, 4414 (1970).

(continued p.153)

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State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{35}\text{Cl}^{16}\text{O}$		$\mu = 10.9749309_5$ $D_0^0 = 2.7505\text{ eV}^a$ I.P. = 11.0 eV^b Several unclassified absorption bands in the region $67000 - 79000\text{ cm}^{-1}$.								SEP 1976 A	
H	(74125)	(1025)	H					H \leftarrow X, V	74212	H	(14)
G ($^2\Pi$)	$\begin{Bmatrix} 73913 \\ 73878 \end{Bmatrix}$	1075	H 10					G \leftarrow X, V	$\begin{Bmatrix} 73705 \\ 73986 \end{Bmatrix}$	H H	(14)*
F ($^2\Sigma$)	69109	[1001] ^c	H					F \leftarrow X, V	$\begin{Bmatrix} 68869 \\ 69181 \end{Bmatrix}$	H H	(14)*
E ($^2\Sigma$)	67333	1070	H 4					E \leftarrow X, V	$\begin{Bmatrix} 67120 \\ 67445 \end{Bmatrix}$	H H	(14)*
D ($^2\Sigma$)	64486	1050	H 2					D \leftarrow X, V	$\begin{Bmatrix} 64269 \\ 64582 \end{Bmatrix}$	H H	(14)*
C ($^2\Sigma$)	58448	1062	H 3					C \leftarrow X, V	$\begin{Bmatrix} 58234 \\ 58554 \end{Bmatrix}$	H H	(14)*
A $^2\Pi_1$	$\begin{Bmatrix} 32169 \\ 31650 \end{Bmatrix}$	519.5	Z 7.2 ^d	0.445_0^e	0.006^f	[1.31]	1.858	A \leftrightarrow X, R	$\begin{Bmatrix} 31682.9^g \\ 31482.3^g \end{Bmatrix}$	Z Z	(1)(2)(3)* (4)* (16)* (17)*
X $^2\Pi_1$	$\begin{Bmatrix} 318^h \\ 0 \end{Bmatrix}$	853.8^i	Z 5.5 ^j	0.62344_8^k	0.0058^l	[1.33]	1.56963	Matrix IR and Raman sp. Microwave sp. ^m EPR sp. ^m			(12)(15) (7)(8) (5)(6)(9)(11)
$(^{35})\text{Cl}^{16}\text{O}^-$		I.P. = 2.5 eV^n									SEP 1976

ClO , ClO^- :

^aFrom the convergence limit of the A \leftarrow X, $^2\Pi_{3/2} \leftarrow ^2\Pi_{1/2}$ subbands (16) assuming dissociation into $^2P_{3/2} + ^1D$.

^bMass-spectrometric studies and theoretical calculations; see (10).

^c $\Delta G(3/2) = 950$, $\Delta G(5/2) = 980$.

^d $w_e v_e = -0.11$; see ^e.

^eIn absorption observed to $v'=25$ of $^2\Pi_{3/2}$ [B_v , D_v values in (16)(17)], close to the dissociation limit at 38052 cm^{-1} above X $^2\Pi_{3/2}(v=0)$. The constants are for levels with $v \leq 9$. All absorption and emission bands are diffuse on account of predissociation. Linewidths in different bands vary from 0.3 to 3.1 cm^{-1} and are $>5 \text{ cm}^{-1}$ in $v'=6$ (16).

ClO , ClO^- (continued):

$$f_{\gamma_e}^i = + 0.000024.$$

^eNote that there have been several changes of vibrational numbering [see, e.g., (13)]; here we have used that of (16) and (17).

^hFrom the VUV absorption spectrum (14); confirmed by EPR spectrum (5)(11).

ⁱThe effective ω_e values for $^2\Pi_{\frac{1}{2}}$ and $^2\Pi_{\frac{3}{2}}$ are 853.0 and 854.9 cm^{-1} , resp. (17).

$$j_{\omega_e \gamma_e}^j = - 0.02.$$

^kFrom combined microwave and ultraviolet data; the microwave values of (8) are $B_0(^2\Pi_{\frac{3}{2}}) = 0.619773$ and $B_0(^2\Pi_{\frac{1}{2}}) = 0.621231$. Λ -type doubling in the $^2\Pi_{\frac{1}{2}}$ component, $\Delta v_{fe} = (+)0.02249(J+\frac{1}{2})$.

$$l_{\gamma_e}^l = + 0.000016.$$

^mDipole moment from Stark effect of microwave spectrum $\mu_{el}(v=0) = 1.239 \text{ D}$ (8), from Stark effect of EPR spectrum 1.18 D (6). eqQ and other hyperfine structure constants in (8)(11).

ⁿIndirectly from thermochemical data and mass-spectrometric studies; also theoretical calculations; see (10).

- (1) Pannetier, Gaydon, *Nature* 161, 242 (1948).
- (2) Porter, DFS 2, 60 (1950).
- (3) Porter, Wright, ZE 56, 782 (1952).
- (4) Durie, Ramsay, CJP 36, 35 (1958).
- (5) Carrington, Dyer, Levy, JCP 47, 1756 (1967).
- (6) Carrington, Levy, Miller, JCP 47, 3801 (1967).
- (7) Amano, Hirota, Morino, JMS 27, 257 (1968).
- (8) Amano, Saito, Hirota, Morino, Johnson, Powell, JMS 30, 275 (1969).
- (9) Uehara, Morino, JMS 36, 158 (1970).
- (10) O'Hare, Wahl, JCP 54, 3770 (1971).
- (11) Uehara, Tanimoto, Morino, MP 22, 799 (1971).
- (12) Andrews, Raymond, JCP 55, 3087 (1971).
- (13) Briggs, *Nature* PS 232, 13 (1972).
- (14) Basco, Morse, JMS 45, 35 (1973).
- (15) Chi, Andrews, JPC 77, 3062 (1973).
- (16) Coxon, Ramsay, CJP 54, 1034 (1976).
- (17) Coxon, Jones, Skolnik, CJP 54, 1043 (1976).

ClF , ClF^+ (continued):

- (7) Anderson, Mamantov, Bull, Grimm, Carver, Carlson, CPL 12, 137 (1971).
- (8) Ewing, Tigelaar, Flygare, JCP 56, 1957 (1972).
- (9) Davis, Muenter, JCP 57, 2836 (1972).
- (10) DeKock, Higginson, Lloyd, Breeze, Cruickshank, Armstrong, MP 24, 1059 (1972).
- (11) Green, JCP 58, 3117 (1973).

- (12) McGurk, Norris, Tigelaar, Flygare, JCP 58, 3118 (1973).
- (13) See ref. (35) of Cl_2 .
- (14) Carroll, Thomas, JCP 60, 2186 (1974).
- (15) Lovas, Tiemann, JPCRD 3, 609 (1974).
- (16) Nordine, JCP 61, 224 (1974).
- (17) Coxon, CPL 33, 136 (1975).
- (18) Janda, Klemperer, Novick, JCP 64, 2698 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^{14}\text{N}$										SEP 1976 A
$\mu = 6.46219329$ $D_0^0 = 7.76 \text{ eV}^a$ I.P. = 14.17 eV^b Theoretical work (24)(46)(48)(50)(63). RKR potential curves (15)(44)(53). Franck-Condon factors (21a)(53), and ref. in (27)(44).										
J $^2\Delta_i$	65258.19 ^c	1121.76	Z 14.203 ^d	1.305 ₂	0.020 ₈	5.8	1.413 ₇	J→A, R	55667.14 ^e Z	(8)*
H $^2\Pi_{(r)}$	[61969.7] ^f			[1.520]			[1.310]	H→B, R	35140.8 ₄ ^e Z	(7)
G $^2\Pi$	[61655.0] ^{g,h}			[1.085] ^g			[1.551]	G→B, R	34826.1 ₀ ^g Z	(7)(43)
F $^2\Delta_r$	60095.6 ₄ ⁱ	1239.5 ₀	Z 12.7 ₅	1.383 ₄	0.0187	7	1.3732	F→A, R	50563.8 ₀ ^e Z	(7)* (22) (47)
E $^2\Sigma^+$	59151.1 ₈	1681.43	Z 3.60 ^j	1.4871	0.0064 ₃ ^k	5.0	1.3245	E→A, R	49842.4 ₇	(8)* (47)
								E↔X, R	58959.85 Z	(8)* (43)*
D $^2\Pi_i$	54486.3 ^l	1004.7 ₁ ^m	Z 8.7 ₈	1.162 ^m	0.013	7	1.498	D→A, R	44838.0 ₈ ^e Z	(7)*
								D→X, R	53955.4 ₆	(7)*
a $^4\Sigma^+$	(32400) ⁿ									
B $^2\Sigma^+$	25752.0	2163.9 ^o	Z 20.2 ^{e'}	1.973 ^o	0.023 ^{e'}	[6.6]	1.150	B→A, V	16680.4 ₆	(31)(54)*
[For a comprehensive review of molecular data on the B-X system including a bibliography of references prior to 1972 see (44)].								B ^p ↔X, ^q v_R	25797.84 Z	(1)* (2)* (4a)(5)(7) (9)(32)(64)
A $^2\Pi_i$	9245.28 ^r	1812.5 ₆ ^s	Z 12.60 ₉ ^t	1.715 ₁ ^s	0.01708 ^u	5.93 ^{sv}	1.2333	A ^w ↔X, ^x R	9117.38 ^e Z	(3)* (3a) (4b)(7)(9) (16)* (28) (32)(44)*
[For a useful compilation of molecular data on the A-X system and a bibliography of references prior to 1971 see (44).]										(62)(70)
X $^2\Sigma^+$	0	2068.59	Z 13.087 ^y	1.8997 ₄ ^z	0.01736 ₉ ^{a'}	6.40 ^{b'}	1.1718 ₂	IR fundamental b. Microwave sp. ^{c'} ESR sp. ^{d'}		(66)(71) (41)(73)

CN: ^aBased on $\Delta H_{f0}^{\circ}(\text{CN}) = 103.2 \pm 2.5$ kcal/mole recommended in (46a). It represents an average value obtained from mass-spectrometric (14) and shock tube studies (10)(13)(39)(56) and from the photo-ionization (25)(33)(37) and -dissociation (35) of CN containing molecules and their decomposition in collisions with Ar metastable atoms (34). The most recent quantitative absorption measurements by (69) together with lifetime measurements in the B-X system (see ^p) tend to support the slightly higher value, $\Delta H_{f0}^{\circ} = 105.5 \pm 2$ kcal/mole, of (37), giving $D_0^0 = 7.6_6$ eV. Gaydon (30) recommends 7.7_5 eV.

^bIndirectly from a combination of photo-ionization (25)(33) and -dissociation (35) threshold energies for HCN and C λ CN; in good agreement with an electron impact appearance potential of 14.2 eV (14). Similar photoionization data for HCN (37) suggest, however, 14.03 eV. Theory predicts 14.10 eV (69a).

^c $A_0 = -26.9_0$, $A_1 = -25.6_7$, $A_2 = -25.4_0$, $A_3 = -24.9_7$; recalculated from (8) with an improved A_0 for A $^2\Pi_1$.

^d $w_{eYe} = +0.180$.

^eRefers to the zero point of the Hill-Van Vleck formula for $\Lambda \neq 0$ states.

^f $A_0 = (+)49.5_7$.

^gVibrational numbering unknown; only the $v' \rightarrow 1$ band at 32702.6_0 cm $^{-1}$ was identified. See also (48).

^h $|A|$ even smaller than in the D state.

ⁱ $A_0 = +28.7_7$, $A_1 = +27.8_6$, $A_2 = +27.0_6$.

^j $w_{eYe} = -1.02$.

^k $r_e = -0.00077$.

^l $A_0 = -3.03$.

^mVibrational numbering uncertain.

ⁿPredicted by ab initio calculations (46)(48). This state is probably responsible for the small perturbation in $v=11$, $N=20$ of B $^2\Sigma^+$ (67); see also (58).

FROM (1); much improved $\Delta G(v+\frac{1}{2})$, B_v , D_v values for $v \leq 7$ in (64), but no equilibrium constants given. Spin-rotation interaction constant $\gamma_0 = +0.01565$ [from the magnetic resonance spectrum (59)], for higher v see (64). Perturbations by A $^2\Pi$ (in $v=0$ at $N=4, 7, 11, 15$; see ^s), and by a $^4\Sigma^+$ (see ⁿ). From Stark effect of the P(1) and R(0) lines in the B-X, 0-0 band (36) determine for the B state $\mu_{el}(\text{CN}^+) = 1.15$ D.

^pRadiative lifetime $\tau(v=0) = 65.6$ ns for the unperturbed levels and 72 ns for the perturbed $N=4$ level [tunable laser excitation (65)]. Phase shift measurements (42) give 59 ns for $v=0-2$, in good agreement with the direct decay measurements, 60.8 ns, of (57). From the zero-electric-field-limit linewidth of the anticrossing spectrum (51) derive 39 ns. The electronic f value for the B-X system at 3860 \AA , $f = 0.033$, is primarily based on shock tube emission and absorption measurements; for a review see (56).

^qFor 0-0, 0-1, 0-2 bands of $^{13}\text{C}^{14}\text{N}$ see (4).

^r $A_v = -52.64 + 0.036_5 v + 0.0086 v^2$, $v \leq 12$ (21).

^sThe vibrational and rotational constants given here are those of (21) based on the measurements of (16); see also (7). More elaborate evaluations, primarily intended to assist in the identification of CN lines in the solar spectrum, have been published by (43a) and (45); note, however, that the constants tabulated in (43a) are not the usual Dunham coefficients. An extension of the system to bands with $v' \leq 25$ (32) requires the use of slightly different vibrational constants.

Λ -type doubling, for details see (3)(21). The rotational perturbations by B $^2\Sigma^+$ in $v=10$ have been the subject of many experimental and theoretical investigations (12)(17); microwave-optical double resonance (11)(18)(19)(29)(38)(40)(52), level anticrossing spectroscopy (49)(51)(60), magnetic (continued p. 156)

CN (continued):

- resonance (59). Hyperfine structure constants in (52),
 $\mu_{e\ell}(^+CN^-) = 0.56 \text{ D}$ (60), $\Pi \vee \Sigma$ interaction parameters (59).
 $t_{we}y_e = -0.0118$.
 $u_{\gamma_e} = -0.000036_4$.
 $v_{\beta_e} = +0.042_5 \times 10^{-6}$.
^wRadiative lifetime $\tau = 0.68 \mu\text{s}$ (average for $1 \leq v \leq 9$),
 corresponding to $f_{00} = 0.0034$ (20), in good agreement with
 (70). A shock tube emission study (55) gives $f_{e\ell} = 0.0045$
 at 10970 \AA . See also (26)(68). A considerably shorter life-
 time for $v=10$, $\tau = 0.14 \mu\text{s}$, was derived by (51) from the
 anticrossing and microwave linewidths. Calculated relative
 absorption coefficients at three different temperatures in
 (61).
^xRotational analyses of the 0-0, 1-0, 2-0, 2-1, 3-1 bands of
 $^{13}\text{C}^{14}\text{N}$ in (23)(72).
^y $w_{ey_e} = -0.00909_3$. Vibrational constants from (7), slightly
 different constants in (21).
^zSpin-splitting constant $\gamma_0 = +0.00725$, from the microwave
 spectrum (66)(71); see also (21)(64). $\mu_{e\ell}(^+CN^-) = 1.45 \text{ D}$
 from Stark effect in the B-X, 0-0 band (36).
^a $\gamma_e = -0.0000310_7$. Rotational constants from (64) who gives
 $\gamma_e = -0.0003107$ which appears to be a misprint; see also
 (7)(21).
^b $\beta_e = +0.01_2 \times 10^{-6}$ (21)(64).
^cIn emission from interstellar sources; eqQ and other hyper-
 fine structure constants.
^dIn rare gas matrices at 4K.
^eThe ΔG and B_v curves are strongly non-linear.

- (1) Jevons, PRS A 112, 407 (1926).
- (2) Jenkins, PR 31, 539 (1928).
- (3) Jenkins, Roots, Mulliken, PR 39, 16 (1932).
- (3a) Parker, PR 41, 274 (1932).
- (4) Jenkins, Wooldridge, PR 53, 137 (1938).
- (4a) White, JCP 8, 79, 459 (1940).
- (4b) Herzberg, Phillips, ApJ 108, 163 (1948).
- (5) Feast, PPS A 62, 121 (1949).
- (6) Kiess, ApJ 109, 551 (1949).
- (7) Douglas, Routly, ApJ(Suppl.) 1, 295 (1955).
- (8) Carroll, CJP 34, 83 (1956).
- (9) Kiess, Broida, JMS 7, 194 (1961).
- (10) Knight, Rink, JCP 35, 199 (1961).
- (11) Barger, Broida, Estin, Radford, PRL 2, 345 (1962).
- (12) Radford, Broida, PR 128, 231 (1962).
- (13) Tsang, Bauer, Cowperthwaite, JCP 36, 1768 (1962).
- (14) Berkowitz, JCP 36, 2533 (1962).
- (15) Fallon, Vanderslice, Cloney, JCP 37, 1097 (1962).
- (16) Davis, Phillips, BAMS 1 (1963).
- (17) Radford, Broida, JCP 38, 644, 3031(Erratum) (1963).
- (18) Evenson, Dunn, Broida, PR A 136, 1566 (1964).
- (19) Radford, PR A 136, 1571 (1964).
- (20) Jeunehomme, JCP 42, 4086 (1965).
- (21) Poletto, Rigutti, NC 39, 519 (1965).
- (21a) Halmann, Laulicht, ApJ(Suppl.) 12, 307 (1966).
- (22) Jha, Rao, PIAS A 63, 316 (1966).

CN (continued):

- (23) Wyller, ApJ 143, 828 (1966).
- (24) Purcell, JCP 47, 1198 (1967); 48, 5735 (1968).
- (25) Dibeler, Liston, JCP 47, 4548 (1967).
- (26) Gippius, Kudryavtsev, Pechenov, Sobolev, HT(USSR) 5, 27 (1967).
- (27) Ortenberg, Antropov, SPU 9, 717 (1967).
- (28) Weinberg, Fishburne, Rao, JMS 22, 406 (1967).
- (29) Evenson, APL 12, 253 (1968).
- (30) Gaydon, DISSEN (1968).
- (31) LeBlanc, JCP 48, 1841 (1968).
- (32) LeBlanc, JCP 48, 1980 (1968).
- (33) Dibeler, Liston, JCP 48, 4765 (1968).
- (34) Setser, Stedman, JCP 49, 467 (1968).
- (35) Davis, Okabe, JCP 49, 5526 (1968).
- (36) Thomson, Dalby, CJP 46, 2815 (1968).
- (37) Berkowitz, Chupka, Walter, JCP 50, 1497 (1969).
- (38) Evenson, PR 178, 1 (1969).
- (39) Levitt, Parsons, TFS 65, 1199 (1969).
- (40) Pratt, Broida, JCP 50, 2181 (1969).
- (41) Easley, Weltner, JCP 52, 197 (1970).
- (42) Liszt, Hesser, ApJ 152, 1101 (1970).
- (43) Lutz, CJP 48, 1192 (1970).
- (43a) Swensson, Benedict, Delbouille, Roland, MSRSL* No. 5 (1970).
- (44) Brocklehurst, Hébert, Innanen, Seel, Nicholls, IAMS 8 (1971); IAMS 9 (1972).
- (45) Fay, Marenin, van Citters, JQSRT 11, 1203 (1971).
- (46) Heil, Schaefer, ApJ 163, 425 (1971).
- (46a) JANAF (1971).
- (47) Lutz, ApJ 164, 213 (1971).
- (48) Schaefer, Heil, JCP 54, 2573 (1971).
- (49) Levy, JCP 56, 5493 (1972).
- (50) Green, JCP 57, 4694 (1972).
- (51) Cook, Levy, JCP 57, 5059 (1972).
- (52) Meakin, Harris, JMS 44, 219 (1972).
- (53) Rao, Lakshman, JQSRT 12, 1063 (1972).
- (54) Schoonveld, JQSRT 12, 1139 (1972); JCP 58, 403 (1973).
- (55) Arnold, Nicholls, JQSRT 12, 1435 (1972).
- (56) Arnold, Nicholls, JQSRT 13, 115 (1973).
- (57) Luk, Bersohn, JCP 58, 2153 (1973).
- (58) Coxon, Setser, Duewer, JCP 58, 2244 (1973).
- (59) Cook, Levy, JCP 58, 3547 (1973).
- (60) Cook, Levy, JCP 59, 2387 (1973).
- (61) Phillips, Leung, ApJ 180, 607 (1973).
- (62) Phillips, ApJ 180, 617 (1973).
- (63) Das, Janis, Wahl, JCP 61, 1274 (1974).
- (64) Engleman, JMS 49, 106 (1974).
- (65) Jackson, JCP 61, 4177 (1974).
- (66) Penzias, Wilson, Jefferts, PRL 32, 701 (1974).
- (67) Coxon, Ramsay, Setser, CJP 53, 1587 (1975).
- (68) Jain, JQSRT 15, 571 (1975).
- (69) Engleman, Rouse, JQSRT 15, 831 (1975).
- (69a) Moffat, JMS 25, 303 (1975).
- (70) Treffers, ApJ 196, 883 (1975).
- (71) Turner, Gammon, ApJ 198, 71 (1975).
- (72) Hosinsky, Lindgren, AA(Suppl.) 25, 1 (1976).
- (73) Adrian, Bowers, CPL 41, 517 (1976).

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{12}\text{C}^{14}\text{N}^+$											
$D_0^0 = 4.8_5 \text{ eV}^a$											
d $^1\Pi$	a+ (46253)	[890.76]	Z	^b	[1.6018]	^c	[19.5] ^c	[1.2762]	d ^d → b, R	37544.49 Z	(1)* (4)*
f $^1\Sigma$	a+45533.6	2670.5	Z	46.9	1.903 ^e	0.032	[4.7]	1.171	f→ b, V	37703.14 Z	(4)*
									f→ a, f	45844.65 Z	(1)*
c $^1\Sigma$	a+ (31771)	(1265) ^g		(11)	(1.403) ^g	(0.002)	[13]	(1.364)	c→ a, R	31381.60 ^g Z	(1)*
b $^1\Pi$	a+8313.6	1688.35	Z	15.12	1.6767	0.0191 ^h	[6.84]	1.2473			
a $^1\Sigma$	a	2033.05	Z	16.14	1.8964	0.0188	[7.0]	1.1729			
$^{12}\text{C}^{14}\text{N}^-$											
$D_0^0 = 10.3_1 \text{ eV}^a$ I.P. = 3.82 eV ^b											
$^{12}\text{C}^{16}\text{O}$											
$\mu = 6.85620871$ $D_0^0 = 11.09_2 \text{ eV}^a$ I.P. = 14.0139 eV ^b											
Absorption in the 100 - 20 \AA region. K absorption of C and O. ^c											
Absorption cross sections from 650 - 180 \AA .											
Several weak and fragmentary progressions in absorption in the region 620 - 530 \AA (161000 - 186000 cm^{-1}), probably corresponding to excitation of two electrons and tentatively assigned as first members of Rydberg series converging to higher electronic states of CO^+ derived from the photoelectron spectrum [revised assignments (125)]. ^d											
Rydberg series ^e converging to B $^2\Sigma^+(v=0)$ of CO^+ (also series or fragments of series with $v'=1, 2$) ^f :											
(nd σ, π)	{	Ogawa and Ogawa's series IV (joining on to R)		{		$v = 158664 - R/(n-0.19)^2$; $n = 3, 4, \dots, 10$.		(101)*			
		Tanaka's diffuse series (joining on to D_2, D_3)		{		$v = 158664 - R/(n-0.55)^2$; $n = 4, 5, \dots, 9$.		(17)* (101)*			
(np σ, π)		Ogawa and Ogawa's series V (joining on to U)		{		$v = 158664 - R/(n-0.61)^2$; $n = 5, 6, 7$.		(101)*			
		Tanaka's sharp series (joining on to S_1, S_2)		{		$v = 158664 - R/(n-0.650-0.084/n-0.13/n^2)^2$; $n = 3, 4, \dots, 13$.		(17)* (101)*			
(ns σ)	{	Ogawa and Ogawa's series III (joining on to T ^g)		{		$v = 158664 - R/(n-0.902-0.232/n)^2$; $n = 4, 5, \dots, 18$.		(101)*			

CN⁺: ^aFrom D₀⁰(CN) and the ionization potentials of CN and C.

^bΔG(3/2) = 548.54, ΔG(5/2) = 542.18, ΔG(7/2) = 550.36.

Vibrational numbering uncertain.

^cB₁ = 1.4319, D₁ = 47.3 × 10⁻⁶;

B₂ = 1.3023, D₂ = 17.9 × 10⁻⁶;

B₃ = 1.2598, D₃ = 19.4 × 10⁻⁶;

B₄ = 1.2196, D₄ = 9 × 10⁻⁶.

Local perturbations in nearly all vibrational levels.

Vibrational numbering uncertain.

^dτ = 24 ns (3).

^ePerturbations; see p. 251 of (2a).

^f0-0 sequence consisting of four headless bands.

^gVibrational numbering uncertain. Homogeneous perturbations by an unidentified state.

^hγ_e = - 0.0005.

(1) Douglas, Routly, ApJ 119, 303 (1954).

(2) See ref. (8) of CN.

(2a) Mulliken, JCP 33, 247 (1960).

(3) Smith, JCP 51, 3410 (1969).

(4) Lutz, ApJ 163, 131 (1971).

(5) See ref. (69a) of CN.

CN⁻: ^aFrom D₀⁰(CN) and the electron affinities of CN and C (1.268 eV).

^bPhotoionization of HCN (1). Earlier measurements are reviewed in this paper. Theory (2) predicts 3.69 eV.

(1) See ref. (37) of CN.

(2) Griffing, Simons, JCP 64, 3610 (1976).

CO: ^aFrom the predissociation in the B ¹Σ⁺ state (see ⁿp.163).

The uncertainty of ±0.017 eV corresponds to the uncertainty as to which combination of ³P component states arises at the dissociation limit.

^bFrom Rydberg series (101). For the second and third I.P. (1π and 4σ orbitals) see the higher Rydberg limits in the Table. The fourth, fifth, and sixth I.P. (3σ, 2σ, 1σ) have been determined from X-ray photoelectron spectroscopy to be 38.9, 296.24 (K limit of C), and 542.57 eV (K limit of O), respectively (62)(78)(162). See also ^f.

^cPreceding the two K limits (see ^b) are strong Rydberg series of absorption bands. The longest-wavelength absorptions correspond to excitation to the 2π orbital yielding a weak ³Π ← X ¹Σ⁺ and a strong ¹Π ← X ¹Σ⁺ peak at 283 and 285 eV for the transitions from 1s_C and at 529 and 532 eV for the transitions from 1s_O (93). The transitions to the ¹Π states have also been observed in electron impact experiments at 287.7 and 534.4 eV (79).

^dDissociation produced by absorption in these bands and subsequent atomic fluorescence (153); predissociation into C⁺ + O⁻ (151).

^eAbsorption and photoionization coefficients from 1000 to 600 Å (33).

^fCalculated Franck-Condon factors for ionization X ²Σ⁺ ← X ¹Σ⁺, A ²Π ← X ¹Σ⁺, and B ²Σ⁺ ← X ¹Σ⁺, see (51) and (53). Observed Franck-Condon factors from photoelectron spectrum (44)(82)(132); absolute ionization cross-sections (113)(161).

^gThe progression P₅ of (17) [called T in MOLSPEC 1 and (40)] must be reclassified as representing the members n=6, 7, and 9 of series III; see the spectrograms of (17) and (101).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{12}\text{C}^{16}\text{O}$ (continued)										
D_3	(153271)	(1705)	(18.5)					$D_3 \leftarrow X$, ^a	153037	(17)* (101)*
U	(153199)	[1676]						$U \leftarrow X$,	152955	(101)*
D_2	(149294)	(1730)	(30)					$D_2 \leftarrow X$, ^a	149070	(17)* (101)*
S_2	(148929)	(1750)	(30)					$S_2 \leftarrow X$,	148715	(17)* (101)*
T	(147065)	(1658)	(11)	e				$T \leftarrow X$,	146810	(101)*
R	(144939)	(1735)	(28)	e				$R \leftarrow X$,	144718	(101)*
S_1	(138038)	(1771)	(29)	e				$S_1 \leftarrow X$,	137835	(101)*
Rydberg series ^b converging to $A^2\Pi(v=0)$ of CO^+ [also series with $v'=1\dots 8$ (Ogawa a. Ogawa) and $v'=1,2,3$ (Tanaka)] ^c :										
(ns σ)		Ogawa and Ogawa's series ^d (joining on to W [$n=3$, see (135)] and O_1, O_2)		}		$\nu = 133484(A^2\Pi_{\frac{1}{2}}) - R/(n-1.077+\dots)^2$; $n = 4,5,\dots,12$.				(101)*
(np σ, π)		Tanaka's α series (joining on to P)		}		$\nu = 133380(A^2\Pi_{\frac{3}{2}}) - R/(n-0.67)^2$; $n = 4,5,\dots,8$.				(17)* (101)
Q	129043	1558	10.6					$Q \leftarrow X$, ^b	R 128738	(17)
$O_2(^1\Pi)$	126729	1560	13.3	e				$O_2 \leftarrow X$,	R 126424	(17)* (101)*
P	123656	[1521]						$P \leftarrow X$,	R 123335	(17)* (101)*
$O_1(^1\Pi)$	121137	1570	13.4	e				$O_1 \leftarrow X$,	R 120837	(4)(101)*
N	(119882)	(1600)		e				$N \leftarrow X$, ^b	(119600)	(4)
Rydberg series ^b converging to $X^2\Sigma^+(v=0)$ of CO^+ [also series with $v'=1$] ^c :										
np π		Ogawa and Ogawa's series ^d (joining on to E, L)		}		$\nu_\infty = 113029$; formula not given, merging into np σ above $n=8$.				(101)*
np σ		Ogawa and Ogawa's series ^d (joining on to C, K)		}		$\nu = 113029 - R/(n-0.615-0.263/n-0.165/n^2)^2$; $n = 3,4,\dots,32$.				(101)*
ns σ		Lindholm's series (joining on to B, J, I')		}		$\nu_\infty = 113029$; formula not given, $n = 3,4,\dots,10$.				(52)
I' (5s σ)								$I' \leftarrow X$,	106383 ^f	(31)* (52)
Z $^1\Sigma^+$				[(1.9)]	(v' unknown)		[(1.1 ₄)]	$Z \leftrightarrow X$, ^b	R 105724 ^g (Z)	(140)
$H^h(^1\Pi)$	(105811)	(1097)	(47)					$H \leftarrow X$, ^{bi}	R 105266	(2)
								Hopfield-Birge ^b .		

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^{16}\text{O}$ (continued)										
$\text{H}^+ 1_{\Pi}$				[1.415]			[1.318]	$\text{H}^+ \leftarrow \text{X}$, R	104119.6 Z	(135)
$\text{L} 1_{\Pi} 4p\pi$	103251	[2181]	(15)	[1.981 ₂]		[14]	[1.114 ₀]	$\text{L} \leftarrow \text{X}$, V	103271.5 Z	(101)* (135)
$\text{L}^+ (1_{\Pi})$								$\text{L}^+ \leftarrow \text{X}$, R	103215 H ^Q	(135)
$\text{K} 1_{\Sigma}^+ 4p\sigma$				[1.918 ₉]		[66]	[1.132 ₀]	$\text{K} \leftarrow \text{X}$, R	103054.3 Z	(101)* (135)
$\text{W} 1_{\Pi} j$				[1.558 ₅]		[65]	[1.256 ₀]	$\text{W} \leftrightarrow \text{X}$, R	102807.1 Z	(135)* (140)
$\text{W}^+ 1_{\Pi}$				[1.536 ₅]			[1.265]	$\text{W}^+ \leftarrow \text{X}$, R	102310.6 Z	(135)*
$\text{J} 1_{\Sigma}^+ 4s\sigma$	(101409)	[2235.3]	Z (15)	[1.9203] ^k		[5.8] ^k	[1.1315] ^k	$\text{J} \leftarrow \text{X}$, R	101456 (Z)	(135)*
$\text{G} 1_{\Pi} (3d\pi)$				[1.9625]		[7.0]	[1.1193]	$\text{G} \leftarrow \text{X}$, V	101031.0 Z	(135)*
$\text{G}^+ 1_{\Pi}$				[(1.59)]	(v' unknown)		[(1.24)]	$\text{G}^+ \leftarrow \text{X}$, R	100651	(135)*
$\text{h} (3_{\Sigma}^+, 4s\sigma)$								$\text{h} \leftarrow \text{X}$, R	100392 (Z)	(135)
$\text{Y} 1_{\Sigma}^+$				[(1.83)]	(v' unknown)		[(1.16)]	$\text{Y} \rightarrow \text{X}$, R	99963 (Z)	(140)
$\text{F} 1_{\Sigma}^+ (3d\sigma)$	(99803)	[2034.4]	Z ^l	[1.86]	^m	[80] ^m	[1.15 ₀]	$\text{F} \leftarrow \text{X}$, ^b R	99739.0 Z	(135)*
								Hopfield-Birge ^b .		
$\text{V} 1_{\Pi}$				[1.70]	(v' unknown)		[1.20]	$\text{V} \leftrightarrow \text{X}$, R	98919.0 H ^Q	(135)(140)

CO: ^aDiffuse looking bands.

^bSee ^e p.159.

^cSee ^f p.159.

^dThese series and progressions from the high resolution work of (101) agree only partially with the early work (17)(18) at lower resolution.

^ePreionization observed in electro-ionization of CO (114).

^fThis strong absorption band is clearly present but not assigned on the spectrogram of (101).

^gAn absorption band at this wavenumber is visible but not identified on the published spectrogram of (101).

^hPreviously called G [see (40)]. The present G 1_{Π} is from (135).

ⁱThis is the strongest system of (2). It is clearly present on the reproduction of (101), but these authors consider the first band at 950 \AA as due to $v'=1$ of $\text{K}(4p\sigma) \leftarrow \text{X}$, do not assign the second (strongest) band at 941 \AA and consider the third band at 933 \AA as $n=5$, $v'=0$ of the Rydberg series which starts with C(3p σ) and E(3p π).
^jcf. Ogawa and Ogawa's Rydberg series converging to A $2_{\Pi_{1/2}}$.
^k $v=0$ diffuse by predissociation, $v=1$ sharp. The rotational constants are for $v=1$ (135).

^l(3a) gives $\omega_e = 2112$, $\omega_e x_e = 198$, presumably from private communication by Hopfield-Birge.

^m $B_1 = 1.837$, $D_1 = 3 \times 10^{-6}$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
12C ¹⁶ O (continued)										
A $^1\Pi$ state at 98836 cm^{-1} reported by (15) was shown (140) to be due to N ₂ .										
g $3\Sigma^+$								g ← X, R 98129.1 Z	(135)	
E $^1\Pi$ 3pπ (92903)	[2153.8]	Z (42)		1.9771 ^a	0.0254	[6.5]	1.1152	E → A, V 28185.18 ^b Z E ← X, ^c V 92930.03 Z Hopfield-Birge b.	(86)* (154) (37)* (135)	
c 3Π 3pπ [93158.5]				[1.935] ^d		[-131] ^e	[1.127]	c → a, V 43603.7 "3A" bands	(57)*	
C $^1\Sigma^+$ 3pσ 91916.5	2175.9 ₂	Z 14.7 ₆ ^f		1.9533 ^g	0.0196	6.2	1.1219	c ← X, V 92076.9 Z C ^h → A, ⁱ V 27174.40 ^b Z Herzberg b. C ^h ↔ X, ^j V 91919.15 Z Hopfield-Birge b.	(64)* (7) (55)(66)	
j ($3\Sigma^+$, 3pσ) 90975	[2166]	Z (15)		[1.8785] ^k	(0.020)	[7.9]	[1.1441]	j ← X, R 90988.04 Z	(55)	
The E ₀ $^1\Sigma^+$ state at 90866 cm^{-1} reported by (15) was shown (140) to be due to N ₂ .										
k [90972]	Single 0-v" progression.							k → a, V 41417 H Kaplan b.	(3)	
B $^1\Sigma^+$ 3sδ 86945.2	2112.7 ₀	Z 15.2 ₂ ^m		1.9612 ⁿ	0.0261	7.1	1.1197	B ^o → A, ^p V 22171.35 ^b Z Ångstrom b. B ^o ↔ X, ^q V 86916.16 Z Hopfield-Birge b.	(7) (55)* (66)	
b $3\Sigma^+$ 3sδ (83814)	[2199.3]	Z		1.986 ^{rs}	0.042		1.113	b ^t → a, ^u V 35358.5 Z 3rd positive gr. ^v b ← X, ^u V 83831.7 H Hopfield-Birge b.	(5)(9)(11) (2)	
(f $3\Sigma^+$)	This state, first suggested by (10) and listed by (40) at T ₀ = 83744, is in all probability not a separate state but represents v = 31 and 35 of a' $3\Sigma^{+w}$									

- CO: ^aClear case of accidental predissociation for $J=31$ (e level) at 94872 cm^{-1} above $v=0$, $J=0$ of $X^1\Sigma^+$ (136).
- ^bThe v_{00} values for $B\rightarrow A$, $C\rightarrow A$, $E\rightarrow A$ are not deperturbed and, therefore, do not add up with the deperturbed v_{00} for $A-X$ (see also ^mp.165) to the v_{00} values listed for $B-X$, $C-X$, and $E-X$.
- ^cOscillator strength $f_{00} = 0.094$ (87).
- ^d Λ -type doubling, $\Delta v = 0.011 \times N(N+1)$. Triplet splitting unobservably small as for most Rydberg states.
- ^e $H_0 = -1.9 \times 10^{-7}$. The rotational constants represent average values for the two Λ -doubling components.
- ^fOnly $v=0$ and 1 observed in absorption, only $v=0$ in emission. w_e , $w_e x_e$ derived with the aid of isotope ($^{12,13}\text{CO}$) data, see (55).
- ^g $\mu_{el} = 4.5\text{ D}$, from Stark effect observations on the Herzberg bands (155).
- ^hLifetime $\tau(v=0) = 1.5\text{ ns}$ (47)(120); electronic branching ratios (120).
- ⁱ(60) and (67) have studied the bands of the isotopic molecules $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$.
- ^jOscillator strength $f_{00} = 0.16_3$ (87).
- ^kRotational lines are diffuse because of predissociation.
- ^lIn the electron energy loss spectrum (144) find a peak at 90858 cm^{-1} which, according to them, cannot be identified with the $j^3\Sigma^+$ state.
- ^mOnly two vibrational levels observed, $\Delta G(\frac{1}{2}) = 2082.26$. w_e , $w_e x_e$ derived with the aid of isotope data (55).
- ⁿA partial breaking off of the rotational structure in the Ångström bands occurs above $J=37$ in $v'=0$ and above $J=17$ in $v'=1$ leading to a dissociation limit at $89595 \pm 30\text{ cm}^{-1}$ (21). RKR potential (40). $\mu_{el} = 1.6_0\text{ D}$ from Stark effect measurements on the Ångström bands (155).

- ^oLifetime $\tau(v=0) = 21.8\text{ ns}$ (100), good agreement with (47)(73)(120). $\tau(v=1) = 15.5\text{ ns}$ (100); (73) give 23.8 ns . Electronic branching ratios (120).
- ^pFranck-Condon factors (40). (75) have studied the rotational structure in the Ångström bands of the isotopic molecules $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{18}\text{O}$ and the perturbations in these isotopes as well as in $^{12}\text{C}^{16}\text{O}$; see also (21)(59).
- ^qOscillator strength $f_{00} = 0.015_3$ (87). Discussion of the r -dependence of the transition moment (100).
- ^rThis state is strongly perturbed by the higher vibrational levels of the $a'^3\Sigma^+$ state (near its dissociation limit). (5) derived $B_0 = 1.89$ from lines with N values between 7 and 15. (6) from deperturbed term values derived $B_0 = 2.058$; (8) gave $\alpha = 0.033$. The listed values of B_e and α_e are from a revised deperturbation by (16) who also gives the deperturbed constants $\Delta G(\frac{1}{2}) = 2188$ and $T_0 = 83816$.
- ^sOnly two vibrational levels, $v=0$ and 1, have been observed. Breaking off on account of predissociation in $v=0$ above $N=55$, in $v=1$ above $N=42$ (6)(9). The absence of $v=2$ is puzzling since it is expected to lie below the dissociation limit (22).
- ^tLifetimes $\tau(v=0) = 53.6\text{ ns}$, $\tau(v=1) = 69.1\text{ ns}$ (74)(118).
- ^uFranck-Condon factors (40).
- ^vThe $b\rightarrow a$ bands with $v'=1$ were previously called "5B" bands (1).
- ^wThis interpretation was first suggested by (12). It is in agreement with the data of (109) on the $a'-X$ system. The occurrence of these particular vibrational levels of $a'^3\Sigma^+$ in the emission spectrum is due to strong interaction with $b^3\Sigma^+$. Indeed, the levels mentioned were observed as "extra" bands accompanying the $b^3\Sigma^+ \rightarrow a^3\Pi$ (third positive) bands.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^{16}\text{O}$ (continued)										
D $^1\Delta$	65928	1094.0	10.20	1.257	0.017		1.399	D \leftarrow X, R 65391 ^a		(43)* (96) (109)
I $^1\Sigma^-$	65084.4 ₀	1092.22	Z 10.70 ₄ ^b	1.2705 ^c	0.01848 ^d	$D_2 = 9.0$	1.3911	I ^e \leftarrow X, R 64546.2 ₆ Z		(39)* (96) (109)*
A $^1\Pi$	65075.7 ₇	1518.2 ₄	Z 19.40 ^f	1.6115 ^g	0.0232 ₅ ^h	7.33 ⁱ	1.2353	A ^j \leftrightarrow X, ^{kl} R 64748.48 ^m Z 4th positive gr.		(63)* (109)*
e $^3\Sigma^-$	64230.2 ₄	1117.7 ₂	Z 10.686 ⁿ	1.2836 ^o	0.01753 ^p	6.77 ^q	1.3840	e \rightarrow a, ^r R 15231.6 Herman b.		(19)* (28)
								e \leftarrow X, R 63704.8 ₅ Z		(23)* (96) (109)*
d $^3\Delta_1$	61120.1 ^s	1171.94	Z 10.635 ^t	1.3108 ^u	0.01782 ^v	6.59 ^q	1.3696	d ^w \rightarrow a, ^r R 12148.7 Triplet b.		(13)(29)(76)
								d \leftarrow X, R 60621.9 ^t Z		(71)(109)*
a' $^3\Sigma^+$	55825.4 ₉	1228.60	Z 10.468 ^x	1.3446 ^y	0.0189 ₂ ^z	6.41 ^q	1.3523	a' $\alpha\rightarrow$ a, ^{β} R 6882.4 Asundi b.		(1)(11)(14)
								a' \leftarrow X, ^{β} R 55355.6 Z Hopfield-Birge b.		(23)* (96) (109)*

CO: ^aExtrapolated, only $v'=1, 6, 21$ observed.

^b $+0.0554(v+\frac{1}{2})^3 - \dots$; for higher order coefficients see (109).

^cRKR potential (109).

^d $+0.00029_1(v+\frac{1}{2})^2 - + \dots$; for higher order coefficients see (109). Revised coefficients from deperturbed B_v values in (98a).

^eLifetime of this state (and/or D $^1\Delta$) $97 \pm 15 \mu\text{s}$ (124).

^f $+0.76_6(v+\frac{1}{2})^3 - + \dots$; higher order coefficients in (109). Because of numerous perturbations (see ^g) these constants do not accurately represent the observed ($v \leq 23$) vibra-

tional levels. Revised coefficients from deperturbed T_v values [see (105)] in (98a).

^gNumerous perturbations produced by e $^3\Sigma^-$, d $^3\Delta$, a' $^3\Sigma^+$, D $^1\Delta$, I $^1\Sigma^-$, discussed by many investigators and summarized in (63). Deperturbed T_v and B_v values are given by (105), see also (98a). RKR potential (109); the potential function has a maximum, the last observed level lies above the dissociation limit.

^h $+0.00159(v+\frac{1}{2})^2 - + \dots$; higher order coefficients in (109), revised coefficients from deperturbed B_v values in (98a).

ⁱCalculated value, $\beta_e = +0.10 \times 10^{-6}$; see (105).

CO: ^jLifetimes for $v=0, \dots, 6$ are 10.7, 10.4, 9.4, 9.0, 9.7, 9.8, 10.5 ns, respectively (47)(89)(99). Values that are about 50% larger were given by (81).

^kOscillator strength $f_{el} = 0.195$, $f_{00} = 0.020$ (87). f values from lifetime measurements (47) are approximately a factor of 2 smaller. See also (91)[r -dependence of electronic transition moment, $f_{el} \approx 0.15$] and (94)(121). Franck-Condon factors (38)(40)(160).

^lSee (27)(116) for spectroscopic data on ^{13}CO and C^{18}O .

^mThis is a nominal, rotationally deperturbed value. The lowest observed levels ($v=0$, $J=1$) lie at 64747.90(-) and at 64748.09(+) which would correspond to a $J=0$ level at 64744.8 cm^{-1} .

ⁿ $+0.117_4(v+\frac{1}{2})^3 - + \dots$; from (109), see also (98a).

^oSpin-splitting constant $\lambda_0 = +0.51$; for its dependence on v see (98a)(131). RKR potential (109).

$P + 7.1 \times 10^{-6}(v+\frac{1}{2})^2 + - \dots$; the coefficients are from (109), but considerably different values for the higher order terms were obtained by (98a) from deperturbed rotational constants.

^qCalculated value, see (98a).

^rIntensity distribution, relative electronic transition moments: $e \rightarrow a$ (156), $d \rightarrow a$ (108). Franck-Condon factors: $d \rightarrow a$ (40). Rotational intensity distribution in the "triplet" bands (36).

^s $A_v = -16.00_5 - 0.113(v+\frac{1}{2}) - 0.0035_7(v+\frac{1}{2})^2$; from (98a).

^t $+0.0785(v+\frac{1}{2})^3 - 0.00163_4(v+\frac{1}{2})^4$. The constants refer to the $^3\Delta_2$ component (109); see also (98a).

^uRKR potential (109).

^v $+0.000113(v+\frac{1}{2})^2$. The constants refer to the $^3\Delta_2$ component (109). From properly averaged term values of $v=3, 4, 7, 9$ (29) gives $B_e = 1.3099$, $\alpha_e = 0.0167_7$, in good agreement with the first two of the expansion coefficients determined by (98a).

^wLifetime strongly dependent on J and Ω because of perturbations by $A^1\Pi$ (117).

^x $+0.0091(v+\frac{1}{2})^3 + 0.00259(v+\frac{1}{2})^4 - + \dots$ (109). Revised coefficients from deperturbed T_v values in (98a).

^ySpin-splitting constants $\lambda_0 = -1.23$, $\gamma_0 \approx -0.007$; dependence on v (98a)(131). See also (143). Dipole moment $\mu_{el} = 1.0_6 \text{ D}$ ($^-\text{CO}^+$), from the radiofrequency spectrum of a $^3\Pi$; see (111)(147). RKR potential (109).

^z $+0.00034_5(v+\frac{1}{2})^2 - + \dots$ (109); revised coefficients from deperturbed B_v values in (98a).

^{\alpha}Lifetime 3.7 to 2.9 μs for $v=5$ to 8 (49).

^{\beta}Franck-Condon factors (38)(40).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^{16}\text{O}$ (continued)										
a $^3\Pi_r$	48686.70 ^a	1743.4 ₁	14.3 ₆ ^b	1.69124 ^c	0.01904 ^d	6.36 ^e	1.20574	a ^f ↔X, ^g R 48473.22 ^b		(20)* (104)
X $^1\Sigma^+$	0	2169.81358 Z	13.28831 ^h	1.93128087 ⁱ	0.01750441 ^j	6.1214 ₇ ^k	1.128323 ^l	Cameron b.		(109)*
								Rot.-vibr. sp. ^{mn} ;		
								3-0		(45)(48)(129)
								2-0 ^o		(139)
								1-0 ^p		(26)(41)
								Rotation sp.;		
								Far IR sp. ^q		(25)
								Microwave sp.		(24)(70)(134)
								Mol. beam el. reson. ^r		(141)
								Mol. beam magn. reson. ^s		(46)(54)

CO: $A_v = +41.53 - 0.14(v+\frac{1}{2}) - 0.009(v+\frac{1}{2})^2$;

$A_J(v=0) = -0.000206$.

$b = 0.04_5(v+\frac{1}{2})^3 + 0.002_5(v+\frac{1}{2})^4$; all vibrational and rotational constants for this state are from deperturbed levels (104) (105).

^cVery precise values for the Λ -type doubling in $^3\Pi_1$ and $^3\Pi_2$, $v=0-7$, $J=1-8$, have been obtained (77)(83)(111)(147) from the study of the radiofrequency spectrum in a molecular beam electric resonance apparatus. While these doublings are small and increase rapidly with J the Λ -doubling for $^3\Pi_0$ [from combination defects (5)(34)] is fairly large at low J ($\sim 1.7 \text{ cm}^{-1}$) and decreases with J . Hyperfine structure in $^{13}\text{C}^{16}\text{O}$ (84). Dipole moment ($^+\text{CO}^-$) from molecular beam electric resonance spectrum $\mu_{e,l}(v=0) = 1.374 \text{ D}$ (111); dipole moment function and radiative lifetimes for vibrational transitions in a $^3\Pi$ (150)(152).

^d $= 0.000041(v+\frac{1}{2})^2$; see ^b.

^eCalculated value, $\beta_e = +0.04 \times 10^{-6}$ (104)(105).

^fLifetime from time of flight studies $\sim 9.5 \text{ ms}$ (112); from afterglow decay 7.5 ms (88)(110); theoretical values (92).

^gFranck-Condon factors (38)(40).

$h + 0.010511(v+\frac{1}{2})^3 + 5.74 \times 10^{-5}(v+\frac{1}{2})^4 + 9.83 \times 10^{-7}(v+\frac{1}{2})^5 - 3.166 \times 10^{-8}(v+\frac{1}{2})^6$; $v \leq 37$ (142).

ⁱRKR potential functions (97)(103)(106).

$j + 5.487 \times 10^{-7}(v+\frac{1}{2})^2 + 2.54 \times 10^{-8}(v+\frac{1}{2})^3$ (142).

$k = 1.153 \times 10^{-9}(v+\frac{1}{2}) + 1.80_5 \times 10^{-10}(v+\frac{1}{2})^2$;

$H_v = [5.83 - 0.1738(v+\frac{1}{2})] \times 10^{-12}$ (142).

^lFrom the effective B_e value; the "true" $B_e = 1.93160$ found by (69) after introducing adiabatic and non-adiabatic corrections (and using older data) leads to $r_e = 1.12823 \text{ Å}$.

See also (102)(122).

^mFor data on $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{18}\text{O}$ see (137)(158).

CO: ⁿ Intensities in 1-0, 2-0, 3-0 rotation-vibration bands and dipole moment function (42)(65)(90)(107)(127)(128)(146)(159); for $\Delta v=1$ transitions with $v=4-10$ (123). Pressure shift and pressure broadening (50)(58)(68)(129)(145)(148). ^o $\Delta v=2$ sequence up to 33-31 in chemiluminescence (61) and flames (139). ^p $\Delta v=1$ sequence up to 37-36 in the CO laser (72)(80)(138); 1-0 band in resonance fluorescence (30)(32).

- CO: (1) Asundi, PRS A 124, 277 (1929).
 (2) Hopfield, Birge, PR 29, 922 (1929).
 (3) Kaplan, PR 35, 1298 (1930).
 (3a) Jevons, "Band Spectra of Diatomic Molecules" (Physical Society, London 1932).
 (4) Henning, AP(Leipzig) 13, 599 (1932).
 (5) Dieke, Mauchly, PR 43, 12 (1933).
 (6) Gerö, ZP 25, 747 (1935).
 (7) Schmid, Gerö, ZP 23, 656 (1935).
 (8) Schmid, Gerö, ZP 26, 198 (1935).
 (9) Gerö, ZP 101, 311 (1936).
 (10) Schmid, Gerö, Nature 140, 508 (1937).
 (11) Beer, ZP 107, 73 (1937).
 (12) Gerö, ZP 109, 216 (1938).
 (13) Gerö, Szabo, AP(Leipzig) 35, 597 (1939).
 (14) Gerö, Lörinczi, ZP 113, 449 (1939).
 (15) Tschulanowsky, JPUSR 1, 341 (1939).
 (16) Stepanov, JPUSR 2, 197 (1940).
 (17) Tanaka, Sci. Pap. IPCR (Tokyo) 32, 447 (1942).
 (18) Takamine, Tanaka, Iwata, Sci. Pap. IPCR (Tokyo) 40, 371 (1943).
 (19) Herman, Herman, JPR 2, 160 (1948).
 (20) Rao, ApJ 110, 304 (1949).

^q Line widths and intensities (56)(95). High pressure gas and liquid far IR absorption spectra in Ar (119); the quadrupole moment derived from this and other experimental and theoretical work [see (126)] is -2.0×10^{-26} esu cm².
^r $\mu_{\text{el}}(v=0, J=0) = 0.10980 \text{ D } (-\text{CO}^+)$; with the dipole moment function of (65) (see ⁿ) this gives 0.1222 D at r_e (141).
^s $g_J = -0.2689_0 \mu_N$ for ¹²C¹⁶O (46);
 $g_J = -0.2569_1 \mu_N$ for ¹³C¹⁶O (54).

- (21) Douglas, Møller, CJP 33, 125 (1955).
 (22) Barrow, Gratzer, Malherbe, PPS A 69, 574 (1956).
 (23) Herzberg, Hugo, CJP 33, 757 (1955).
 (24) Rosenblum, Nethercot, Townes, PR 109, 400 (1958).
 (25) Loewenstein, JOSA 50, 1163 (1960).
 (26) Rank, Skorinko, Eastman, Rao, Wiggins, JMS 4, 518 (1960).
 (27) Shvangiradze, Oganezov, Chikhladze, OS(Engl. Transl.) 8, 239 (1960).
 (28) Barrow, Nature 189, 480 (1961).
 (29) Carroll, JCP 36, 2861 (1962).
 (30) Millikan, JCP 38, 2855 (1963).
 (31) Huffman, Larrabee, Tanaka, JCP 40, 2261 (1964).
 (32) McCaa, Williams, JOSA 54, 326 (1964).
 (33) Cook, Metzger, Ogawa, CJP 43, 1706 (1965).
 (34) Freund, Klemperer, JCP 43, 2422 (1965).
 (35) Kovács, APH 18, 107 (1965).
 (36) Kovács, Törös, APH 18, 101 (1965).
 (37) Tilford, Vanderslice, Wilkinson, CJP 43, 450 (1965).
 (38) Halmann, Laulicht, ApJ(Suppl.) 12, 307 (1966).
 (39) Herzberg, Simmons, Bass, Tilford, CJP 44, 3039 (1966).
 (40) Krupenie, "The Band Spectrum of Carbon Monoxide", NSRDS-NBS 5 (1966).
 (continued p. 168)

CO (continued):

- (41) Rao, Humphreys, Rank, "Wavelength Standards in the Infrared". Academic Press (1966).
- (42) Young, Eachus, JCP 44, 4195 (1966).
- (43) Simmons, Tilford, JCP 45, 2965 (1966).
- (44) Turner, May, JCP 45, 471 (1966).
- (45) Bouanich, Lévy, Haeusler, CR B 264, 944 (1967).
- (46) Ozier, Yi, Khoshla, Ramsey, JCP 46, 1530 (1967).
- (47) Hesser, JCP 48, 2518 (1968).
- (48) Bouanich, Lévy, Haeusler, JP(Paris) 29, 641 (1968).
- (49) Hartfuss, Schmillen, ZN 23 a, 722 (1968).
- (50) Hunt, Toth, Plyler, JCP 49, 3909 (1968).
- (51) Krupenie, Benesch, JRNBS A 72, 495 (1968).
- (52) Lindholm, AF 40, 103 (1969).
- (53) Nicholls, JP B 1, 1192 (1968).
- (54) Ozier, Crapo, Ramsey, JCP 49, 2314 (1968).
- (55) Tilford, Vanderslice, JMS 26, 419 (1968).
- (56) Dowling, JQSRT 9, 1613 (1969).
- (57) Ginter, Tilford, JMS 31, 292 (1969).
- (58) Hoover, Williams, JOSA 59, 28 (1969).
- (59) Janjić, Pešić, Janković, GHDB 34, 301 (1969).
- (60) Kepa, APP A 36, 1109 (1969).
- (61) Schwartz, Thrush, JMS 32, 343 (1969).
- (62) Siegbahn, Nordling, Johansson, Hedman, Hedén, Hamrin, Gelius, Bergmark, Werme, Manne, Baer, "ESCA Applied to Free Molecules". North-Holland, Amsterdam (1969).
- (63) Simmons, Bass, Tilford, ApJ 155, 345 (1969).
- (64) Tilford, JCP 50, 3126 (1969).
- (65) Toth, Hunt, Plyler, JMS 32, 85 (1969).
- (66) Aarts, de Heer, JCP 52, 5354 (1970).
- (67) Asundi, Dhumwad, Patwardhan, JMS 34, 528 (1970).
- (68) Bouanich, Larvor, Haeusler, CR B 269, 1238; 270, 396, 1220 (1970).
- (69) Bunker, JMS 35, 306 (1970); 37, 197 (1971) (erratum).
- (70) Helming, De Lucia, Gordy, PRL 25, 1397 (1970).
- (71) Herzberg, Hugo, Tilford, Simmons, CJP 48, 3004 (1970).
- (72) Mantz, Nichols, Alpert, Rao, JMS 35, 325 (1970).
- (73) Rogers, Anderson, JOSA 60, 278 (1970).
- (74) Rogers, Anderson, JQSRT 10, 515 (1970).
- (75) Rytel, et al., APP A 37, 559, 585; 38, 299 (1970); 39, 29 (1971); 41, 377, 757 (1972).
- (76) Slinger, Black, CPL 4, 558 (1970).
- (77) Stern, Gammon, Lesk, Freund, Klemperer, JCP 52, 3467 (1970).
- (78) Thomas, JCP 53, 1744 (1970).
- (79) Van der Wiel, El-Sherbini, Brion, CPL 7, 161 (1970).
- (80) Yardley, JMS 35, 314 (1970).
- (81) Chervenak, Anderson, JOSA 61, 952 (1971).
- (82) Comes, Speier, ZN 26 a, 1998 (1971).
- (83) Gammon, Stern, Klemperer, JCP 54, 2151 (1971).
- (84) Gammon, Stern, Lesk, Wicke, Klemperer, JCP 54, 2136 (1971).
- (85) Hasson, Nicholls, JP B 4, 681 (1971).
- (86) Kepa, Rytel, APP A 39, 629 (1971).
- (87) Lassettre, Skerbele, JCP 54, 1597 (1971).
- (88) Lawrence, CPL 9, 575 (1971).
- (89) Imhof, Read, CPL 11, 326 (1971).
- (90) Moskalenko, Mirumyants, SPJ (1973), 721.
- (91) Mumma, Stone, Zipf, JCP 54, 2627 (1971).
- (92) James, JCP 55, 4118 (1971).
- (93) Nakamura, Morioka, Hayaishi, Ishiguro, Sasanuma, 3rd International Conference on Vacuum Ultraviolet Radiation Physics (Tokyo, August 30 - September 2, 1971), paper 1pA1-6.

CO (continued):

- (94) Pilling, Bass, Braun, JQSRT 11, 1593 (1971).
(95) Sanderson, Scott, White, JMS 38, 252 (1971).
(96) Simmons, Tilford, JRNBS A 75, 455 (1971).
(97) Mantz, Watson, Rao, Albritton, Schmeltekopf, Zare, JMS 39, 180 (1971).
(98) James, JMS 40, 545 (1971).
(98a) R. W. Field, Thesis (Harvard University, 1971).
(99) Burnham, Isler, Wells, PR A 6, 1327 (1972).
(100) Imhof, Read, Beckett, JP B 5, 896 (1972).
(101) Ogawa, Ogawa, JMS 41, 393 (1972).
(102) Bunker, JMS 42, 478 (1972).
(103) Dickinson, JMS 44, 183 (1972).
(104) Field, Tilford, Howard, Simmons, JMS 44, 347 (1972).
(105) Field, Wicke, Simmons, Tilford, JMS 44, 383 (1972).
(106) Fleming, Rao, JMS 44, 189 (1972).
(107) Roux, Effantin, d'Incan, JQSRT 12, 97 (1972).
(108) Slanger, Black, JP B 5, 1988 (1972).
(109) Tilford, Simmons, JPCRD 1, 147 (1972).
(110) Wauchop, Broida, JCP 56, 330 (1972).
(111) Wicke, Field, Klemperer, JCP 56, 5758 (1972).
(112) Johnson, JCP 57, 576 (1972).
(113) Judge, Lee, JCP 57, 455 (1972).
(114) Carbonneau, Marmet, CJP 51, 2202 (1973).
(115) Lee, Carlson, Judge, Ogawa, JQSRT 13, 1023 (1973).
(116) Rytel, Siwiec, APP A 44, 67 (1973).
(117) Slanger, Black, JCP 58, 194 (1973).
(118) Smith, Imhof, Read, JP B 6, 1333 (1973).
(119) Buontempo, Cunsolo, Jacucci, JCP 59, 3750 (1973).
(120) Dotchin, Chupp, Pegg, JCP 59, 3960 (1973).
(121) Vargin, Pasynkova, Trekhov, JAS 13, 1340 (1973).
(122) Watson, JMS 45, 99; 48, 479 (1973).
(123) Weisbach, Chackerian, JCP 59, 4272 (1973).
(124) Wells, Borst, Zipf, PR A 8, 2463 (1973).
(125) Åsbrink, Fridh, Lindholm, Codling, PS 10, 183 (1974).
(126) Billingsley, Krauss, JCP 60, 2767 (1974).
(127) Billingsley, Krauss, JCP 60, 4130 (1974).
(128) Bouanich, Brodbeck, JQSRT 14, 1199 (1974).
(129) Bouanich, Brodbeck, RPA 2, 475 (1974).
(130) Codling, Potts, JP B 7, 163, 314 (1974).
(131) Field, Lefebvre-Brion, APH 35, 51 (1974).
(132) Gardner, Samson, JCP 60, 3711 (1974).
(133) Klump, Lassette, JCP 60, 4830 (1974).
(134) Lovas, Krupenie, JPCRD 3, 245 (1974).
(135) Ogawa, Ogawa, JMS 49, 454 (1974).
(136) Simmons, Tilford, JMS 49, 167 (1974).
(137) Johns, McKellar, Weitz, JMS 51, 539 (1974).
(138) Kildal, Eng, Ross, JMS 53, 479 (1974).
(139) Mantz, Maillard, JMS 53, 466 (1974).
(140) Tilford, Simmons, JMS 53, 436 (1974).
(141) Muentert, JMS 55, 490 (1975).
(142) Mantz, Maillard, Roh, Rao, JMS 57, 155 (1975).
(143) Sink, Lefebvre-Brion, Hall, JCP 62, 1802 (1975).
(144) Swanson, Celotta, Kuyatt, Cooper, JCP 62, 4880 (1975).
(145) Varanasi, JQSRT 15, 191 (1975).
(146) Varanasi, Sarangi, JQSRT 15, 473 (1975).
(147) Wicke, Klemperer, Field, JCP 62, 3544 (1975).
(148) Moskalenko, OS(Engl. Transl.) 38, 382 (1975).
(149) Watson, Stewart, Gardner, Lynch, PSS 23, 384 (1975).
(150) Wicke, Klemperer, MP 30, 1021 (1975).
(151) Loch, Dürer, CPL 34, 508 (1975).
(152) Wicke, Klemperer, JCP 63, 3756 (1975).
(153) Lee, Carlson, Judge, Ogawa, JCP 63, 3987 (1975).
(154) Kepa, Knot-Wisniewska, Rytel, APP A 48, 819 (1975).
(continued p.171)

CO⁺, CO⁺⁺;

^a $D_0^0(\text{CO}) + \text{I.P.}(\text{C}) - \text{I.P.}(\text{CO})$.

^bFrom the electron impact appearance potential of CO⁺⁺ in CO (8)(22a), reduced by 0.9 eV following (24); see also ^w.

^cSeveral higher lying states corresponding to excitation of a second electron have been observed by (34) ("ls shake-up spectrum").

^dFairly long progressions in the photoelectron spectrum; vibrational numbering uncertain. Predissociation into C⁺ + O (38)

^e $A \approx +100$.

^fVibrational numbering uncertain; rotational structure not fully resolved.

^g $w_e y_e = +0.328_3$.

^hSpin-splitting constant $\gamma \approx +0.018$.

ⁱRRK potential functions (10)(14)(15).

^j $\beta_e = +0.2_2 \times 10^{-6}$.

^kLifetime $\tau(v=0) = 55 \pm 4$ ns (17)(20)(31)(37), slight increase with v (17)(31). Electronic branching ratio $A(B \rightarrow A) = 0.08/\tau(B)$, $A(B \rightarrow X) = 0.92/\tau(B)$ (29); $f_{00}(B-A) \approx 0.0007_1$, $f_{00}(B-X) \approx 0.0065$.

^lFluorescence by photoexcitation from the ground state X $1\Sigma^+$ of CO (29)(33).

^mFranck-Condon factors (9)(11)(14)(19)(23). Independence of electronic transition moment on r (29)(30); see, however, (6)(13)(28).

ⁿIsotopic bands (7)(34a).

^o $A = -117.5$.

^pVibrational numbering confirmed by isotope studies (22).

^q $w_e y_e = +0.013_1$.

^rLifetimes $\tau(v=1) = 3.4_9$ μs , $\tau(v=3) = 2.7_8$ μs , $\tau(v=4) = 2.6_3$ μs , $\tau(v=6) = 2.4_1$ μs (27). (26) give values that are 10 to 50 % higher; earlier values (5)(18) are 20 % lower.

^sRefers to zero point of Hill - Van Vleck formula.

^t $w_e y_e = -0.000_7$.

^uFrom the microwave spectrum $B_0 = 1.967465$, spin-splitting constant $\gamma_0 = +0.009105$.

^vRough estimate based on appearance potentials of CO⁺⁺ from CO (8)(22a), and taking into account tentative assignments of the carbon and oxygen Auger spectra of CO (21a)(24).

^wThe potential minimum of the ground state of CO⁺⁺ lies about 4.7 eV above the dissociation limit C⁺($^2P_{3/2}$) + O⁺(4S) (which lies 35.97₀ eV above the ground state of CO) and is separated by a maximum of ~ 1.5 eV from this limit (22a)(24).

^xDerived by (24) from the carbon Auger spectrum of CO (21a). At least six vibrational levels are observed.

References on page 173.

CO (continued):

(155) Fisher, Dalby, CJP 54, 258 (1976).

(156) Slinger, Black, JCP 64, 219 (1976).

(157) Wight, Van der Wiel, Brion, JP B 2, 675 (1976)

(158) Chen, Rao, McDowell, JMS 61, 71 (1976)

(159) Tipping, JMS 61, 272 (1976).

(160) Shimauchi, SL 25, 1 (1976).

(161) Samson, Gardner, JESRP 8, 35 (1976).

(162) Smith, Thomas, JESRP 8, 45 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^{16}\text{O}^-$										
				$D_0^0 = 8.1_3 \text{ eV}^a$		I.P. = - 1.5 eV				OCT 1976 A
F		1730	40					b	13.95 eV ^c	(4)(6)
E								d	12.2 eV ^c	(3)(4)(6)
D								d	11.3 eV ^c	(3)(4)(6)
C	$\left\{ \begin{array}{l} 2\Pi \\ 2\Sigma^+ \end{array} \right.$								10.7 eV ^c	(2)(3)(4)(6)
									10.42 eV ^c	(2)(4)(6)
B	$2\Sigma^+$	[1940]						e	10.04 eV ^c	(2)(3)(4)(6)
A		Resonances coincident with the vibrational levels $v=0, 1, 2$ of $a^3\Pi$ of CO, ascribed to a state of CO^- with the same potential function as $a^3\Pi$.							6.0 eV ^c	(7)
X	2Π	Very broad resonance, vibrational structure barely detectable.							1.5 eV ^c	(1)

CO^- : ^aFrom $D_0^0(\text{CO})$ and the electron affinities of CO (-1.5 eV) and O (+1.465 eV).

^bProgression of six resonances, observed in electron transmission (4) and electroionization (5) experiments; vibrational numbering uncertain. Its "grandparent" is assumed to be the A 2Π state of CO^+ , with the additional two electrons in a Rydberg orbital.

^cEnergies in eV above X $1\Sigma^+(v=0)$ of CO, all obtained as resonances in electron scattering experiments.

^dResonances in the excitation functions of CO, B $1\Sigma^+$ and b $3\Sigma^+$ (3), and in the electron transmission current (4).

^eSharp resonance (width ~0.045 eV); $v'=0$ and 1. The parent states are b $3\Sigma^+$ and B $1\Sigma^+$ of CO. Decay into $\text{CO}(X^1\Sigma, a^3\Pi, a^3\Sigma, A^1\Pi) + e^-$, $\text{C} + \text{O}^-$, and $\text{C}^- + \text{O}$; see also (8).

(1) Boness, Hasted, Larkin, PRS A 305, 493 (1968).

(2) Comer, Read, JP B 4, 1678 (1971).

(3) Mazeau, Gresteau, Joyez, Reinhardt, Hall, JP B 5, 1890 (1972).

(4) Sanche, Schulz, PR A 6, 69 (1972).

(5) See ref. (114) of CO.

(6) Schulz, RMP 45, 423 (1973).

(7) Wong, Schulz, PRL 33, 134 (1974).

(8) See ref. (144) of CO.

CO⁺, CO⁺⁺:

- (1) Bulthuis, Physica 1, 873 (1934).
- (2) Rao, ApJ 111, 50 (1950).
- (3) Rao, ApJ 111, 306 (1950).
- (4) Rao, Sarma, MSRSL (4) 13, 141 (1953).
- (5) Bennett, Dalby, JCP 32, 1111 (1960).
- (6) Robinson, Nicholls, PPS 75, 817 (1960).
- (7) See ref. (27) of CO.
- (8) Dorman, Morrison, JCP 35, 575 (1961).
- (9) Nicholls, CJP 40, 1772 (1962).
- (10) Krupenie, Weissman, JCP 43, 1529 (1965).
- (11) See ref. (38) of CO.
- (12) Hesser, Dressler, JCP 45, 3149 (1966).
- (13) Joshi, Sastri, Parthasarathi, JQSRT 6, 215 (1966).
- (14) See ref. (40) of CO.
- (15) Singh, Rai, JMS 19, 424 (1966).
- (16) Herzberg, CPAS 2 (15), 1 (1968).
- (17) See ref. (47) of CO.
- (18) Fink, Welge, ZN 23 a, 358 (1968).
- (19) See ref. (51) of CO.
- (20) Fowler, Skwerski, Anderson, Copeland, Holzberlein, JCP 50, 4133 (1969).
- (21) Marchand, d'Incan, Janin, SA A 25, 605 (1969).
- (21a) See ref. (62) of CO.
- (22) See ref. (67) of CO.
- (22a) Newton, Sciamanna, JCP 53, 132 (1970).
- (22b) See ref. (78) of CO.
- (23) See ref. (82) of CO.
- (24) Hurley, JCP 54, 3656 (1971).
- (25) See ref. (93) of CO.
- (26) Anderson, Sutherland, Frey, JOSA 62, 1127 (1972).
- (27) Holland, Maier, JCP 56, 5229 (1972).
- (28) Jain, JP B 5, 199 (1972).
- (29) See ref. (113) of CO.
- (30) Maier, Holland, JP B 5, L118 (1972).
- (31) See ref. (120) of CO.
- (32) See ref. (125) of CO.
- (33) Lee, Carlson, Judge, Ogawa, JGR 72, 5286 (1974).
- (34) Gelius, JESRP 5, 985 (1974).
- (34a) Pešić, Janjić, Marković, Rytel, Siwiec, GHDB 39, 249 (1974); Pešić, Marković, Janković, Fizika 7, 83 (1975).
- (35) Dixon, Woods, PRL 34, 61 (1975).
- (36) Gardner, Samson, JCP 62, 1447 (1975).
- (37) Jørgensen, Sørensen, JCP 62, 2550 (1975).
- (38) See ref. (151) of CO.
- (39) Lee, Carlson, Judge, JP B 9, 855 (1976).
- (40) See ref. (162) of CO.

System	ν_e	ω_e^I	$\omega_e^I x_e^I$	ω_e^{II}	$\omega_e^{II} x_e^{II}$	Description			References
							Degrad.	ν_{00}	
$^{59}\text{Co}_2$		$\mu = 29.466594_0 \quad D_0^0 = 1.6_9 \text{ eV}^a$							DEC 1974
$^{59}\text{Co}^{(79)}\text{Br}$		$(\mu = 33.738539_1)$ Emission bands in the visible (1)(2) and photographic infrared (4) regions. Tentative assignments:							DEC 1974
System A:	23049.8	269.1	0.4	271.6	- 0.0 ₅	Single heads of line-like app.		23048.4	(3)
" B:	22252.6	304.3	0.7 ₅	318.3	2.1	Single heads	R	22245.9	(3)
" C:	22132.1	306.8	1.6 ₅	324.0	1.5	" "	R	22123.5	(3)
" D:	21731.1	300.2	H ^Q - 0.7 ₂	322.8	0.1 ₅	Double heads	R	21720.0	H ^Q (3)
" E:	21111.5	306.3	H ^Q 1.6	332.7	2.2	" "	R	21098.4	H ^Q (5)
" F:	20712.3	309.0	2.8	332.7	1.95	Single heads	R	20700.4	(5)
" G:	18354.5	317.0	H ^Q 1.6	329.5	2.55	Double heads	R	18348.5	H ^Q (5)
" H:	17927.8	329.3	0.3	337.5	0.2	Single heads	R	17923.7	(5)
" I:	17863.7	326.5	0.8	336.0	0.25	" "	R	17858.8	(5)
" N ₁ :	13831.4	331.3	1.35	316.4	0.88	" "	R	13838.7	(4)
" N ₂ :	13740.5	332.2	H ^Q 1.40	313.9	0.50	Double heads	R	13749.4	H ^Q (4)
$^{59}\text{Co}^{(35)}\text{Cl}$		$(\mu = 21.9465518) \quad D_0^0 = 4.0 \text{ eV}^a$							DEC 1974
The following classification (1)(5) of emission bands [see also (2)] should be considered as tentative only:									
System A:	22967.3 ^b	420.0	1.66	421.8	1.34	Single heads	R	22966.3	(1)
" B:	22404.3 ^b	416.6	0.82	419.4	0.28	" "	R	22402.8	(1)
" C:	22190	401.0		416.2		" "		22182.5	(4)
" D:	22075	410.2		416.4		" "		22072.3	(4)
" E:	22014.6 ^b	420.0	1.14	421.2	0.74	" "	R	22013.9	(1)
" F:	21641	408.0		409.0	- 0.45	" "	R	21640.4	(5)
" G:	21343.0	391.2	2.15	407.1	2.55	" "	R	21335.1	(5)
" H:	21266.1	413.2	2.00	416.8	0.38	" "	R	21263.9	(5)

System	ν_e	ω_e'	$\omega_e'x_e'$	ω_e''	$\omega_e''x_e''$	Description			References
							Degrad.	ν_{00}	

$^{59}\text{Co}(^{35})\text{Cl}$ (continued)									
System I:	20971	405.0	0.80	409.0		Single heads	R	20969.1	(5)
" J:	19957	408.6 H^Q	- 1.00	431.0		Double heads	R	19945.8 H^Q	(5)
" K:	19878	408.4 H^Q	- 0.50	428.0		" "	R	19868.1 H^Q	(5)
" L:		0-0 sequence only.				" "	R	19826.3 H^Q	(5)
	17641							17638.8	
	17558							17555.9	
" M:	17486	412.3		416.0		Multiple heads		17484.1	(3)
	17413							17411.0	
	17330							17328.0	
" N_1 :	14054.0	462.5 H^Q	2.65	482.6	3.65	Double heads	R	14044.2 H^Q	(5)
" N_2 :	13946.1	467.6 H^Q	1.25	484.3	0.90	" "	R	13937.7 H^Q	(5)
" O:	12693.4	478.8	1.38	498.4	- 1.05	" "	R	12683.0	(5)

Co_2 : ^aThermochemical value (mass-spectrom.)(1).
(1) Kant, Strauss, JCP 41, 3806 (1964).

CoBr : (1) Mesnage, CR 204, 1929 (1937).
(2) Mesnage, AP(Paris) 12, 5 (1939).
(3) Rao, Rao, IJP 36, 609 (1962).
(4) Rao, Rao, CS 37, 608 (1968).
(5) Rao, Reddy, Rao, IJPAP 10, 389 (1972).

CoCl : ^aFrom the heat of formation of CoCl(g) reported by (6).

^bThese three band systems may be the three components of a triplet transition.

(1) More, PR 54, 122 (1938).
(2) See ref. (2) of CoBr .
(3) Krishnamurty, CS 20, 323 (1951); IJP 26, 177 (1952).
(4) Krishnamurty, quoted in (5).
(5) Rao, Rao, IJP 35, 556 (1961).
(6) Kulkarni, Dadape, HTS 3, 277 (1971).

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State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{59}\text{Co}(^{63})\text{Cu}$		$(\mu = 30.432929_6)$		$D_0^0 = 1.6_2 \text{ eV}^a$						DEC 1974
$^{59}\text{Co}(^{74})\text{Ge}$		$(\mu = 32.790873_4)$		$D_0^0 = 2.4_3 \text{ eV}^a$						DEC 1974
$^{59}\text{Co}^1\text{H}$		$\mu = 0.99088003$								DEC 1974
A_2 A_1 $\Omega = 4^a$ X_2 X_1 $\Omega = 4^a$ 0			$[1527.8] \text{ z}^b$	6.701^c	0.305	$[6.20]^d$	1.593_4	$A_2 \leftrightarrow X_2, R \text{ 21982 H}$ $A_1 \rightarrow X_1, R \text{ 22243.3}^b \text{ Z}$		(6) (1)* (2)*
				$[7.151]$		$[4.05]$	$[1.542_4]$			
$^{59}\text{Co}^2\text{H}$		$\mu = 1.94754294$		$D_0^0 = (3.2) \text{ eV}$						DEC 1974
A_2 $\Omega = 3^a$ A_1 $\Omega = 4^a$ 22367.4 X_2 $\Omega = 3^a$ x_2^i X_1 $\Omega = 4^a$ 0			$[1110.39] \text{ z}^b$ 1180.9 z^b 32.7	3.4312^e 3.394^g $[3.7559]^j$ 3.7571	0.1059 0.106 0.0747^k	$[1.270]^f$ 1.0^h $[1.223]$ $[1.125]^l$	1.5883_0 1.597_0 $[1.5181]$ 1.5178_5	$A_2 \leftrightarrow X_2, R \text{ 21929.19}^b \text{ Z}$ $A_1 \leftrightarrow X_1, R \text{ 22267.5}^b \text{ Z}$		(5)* (6) (3)(4)* (6)*
			1373.22 z^b 17.59							
$^{59}\text{Co}^{16}\text{O}$		$\mu = 12.5804777_6$		$D_0^0 = 3.8_1 \text{ eV}^a$						DEC 1974
				R shaded bands in emission from 10900 to 15900 cm^{-1} , suggesting $w_e'' = 850$, $w_e'' x_e'' = 6$.						(1)(2)
$^{59}\text{Co}(^{32})\text{S}$		$(\mu = 20.7272512)$		$D_0^0 = 3.3_9 \text{ eV}^a$						DEC 1974
$^{59}\text{Co}(^{28})\text{Si}$		$(\mu = 18.9709743)$		$D_0^0 = 2.8_1 \text{ eV}^a$						DEC 1974

CoCu: ^aThermochemical value (mass-spectrom.)(1).

(1) Kant, Strauss, Lin, JCP 52, 2384 (1970).

CoGe: ^aThermochemical value (mass-spectrom.)(1).

(1) Kant, Strauss, JCP 49, 3579 (1968).

Co¹H, Co²H:

^aPossibly $3\phi_4$ and $3\phi_3$; $3\phi_2$ not identified.

^bContrary to the definitions adopted in these tables the band origins here do not include the J-independent terms $-\Omega^2 B_v$ of the rotational energy expressions for the upper and lower states; the zero lines are obtained by adding $-\Omega^2(B_v' - B_v'')$ to the values given in the table. Heimer (1)(2) uses a different definition.

^c $v=0$ perturbed from $J \approx 10$ to $J \approx 20$.

^d $D_1 = 5.90 \times 10^{-4}$.

^e Ω -type doubling $\Delta v \left\{ \begin{array}{l} (v=0) = 0.36 \\ (v=1) = 0.45 \end{array} \right\} \times 10^{-8} J^6$.

^f $D_1 = 1.326 \times 10^{-4}$.

^gPerturbations in all three observed vibrational levels (4).

^h $\beta_e = + 0.2 \times 10^{-4}$.

ⁱ $x_2 \approx 800 \text{ cm}^{-1}$, estimated from the difference $B_0(\Omega=3) - B_0(\Omega=4)$.

^jConstants derived from the upper Ω -type doubling component; $\Delta v = 3.42 \times 10^{-8} J^6 + \dots$

^k $\gamma_e = - 0.0013$.

^l $H_0 = + 2.56 \times 10^{-9}$; $D_1 = 1.157 \times 10^{-4}$, $H_1 = + 5.9 \times 10^{-9}$;

$D_2 = 1.09 \times 10^{-4}$.

Co¹H, Co²H (continued):

(1) Heimer, Dissertation (Stockholm, 1937).

(2) Heimer, ZP 104, 448 (1937).

(3) Klynning, Neuhaus, ZN 18 a, 1142 (1963).

(4) Klynning, Kronekvist, PS 6, 61 (1972).

(5) Klynning, Kronekvist, PS 7, 72 (1973).

(6) Smith, PRS A 332, 113 (1973).

CoO: ^aThermochemical value (mass-spectrom.)(3), recalculated (4)].

(1) Malet, Rosen, BSRSL 14, 382 (1945).

(2) Rosen, Nature 156, 570 (1945).

(3) Grimley, Burns, Inghram, JCP 45, 4158 (1966).

(4) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

CoS: ^aThermochemical value (mass-spectrom.)(1).

(1) Drowart, Pattoret, Smoes, PBCS No.8, 67 (1967).

CoSi: ^aThermochemical value (mass-spectrom.)(1).

(1) Vander Auwera-Mahieu, McIntyre, Drowart, CPL 4, 198 (1969).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{12}\text{C}^{31}\text{P}$		$\mu = 8.64911823$ $D_0^0 = 5.28 \text{ eV}^a$								OCT 1976 A
B	$2\Sigma^+$	29100.4	836.32 H 5.917	0.6829 ^{bc}	0.00628	(1.82)	1.689 ₄	B→A, R 21934.3 H 22092.6 H		(1)*
								B→X, ^d R 28898.9 H		(1)*
A	$2\Pi_1$	7053.2 6894.9	1061.99 H ^Q 6.035	0.713 ₅ ^e	0.0058 ^e	(1.3)	1.65 ₃			
X	$2\Sigma^+$	0	1239.67 H 6.86	0.7986 ^{fc}	0.00597	(1.33)	1.562 ₂			
$^{(52)}\text{Cr}_2$		$(\mu = 25.970255_1)$ $D_0^0 = 1.5_6 \text{ eV}^a$ A rotationally resolved absorption band at 21751 cm^{-1} was observed in the photolysis of $\text{Cr}(\text{CO})_6$ and could possibly be due to Cr_2 .								DEC 1974 (2)

CP: ^aThermochemical value (mass-spectrom.) (5)(6)(7).
^bSpin-splitting constant $\gamma = (-)0.006$.
^cRKR potential curves (2).
^dMorse-potential Franck-Condon factors (4).
^eRecalculated from head-head separations in the B-A system. Similar calculations by (1) gave $B_e = 0.698$, $\alpha_e = 0.0077$. The rotational analysis of the B-A, 0-0 band (3) yields $B_0 = 0.7101$.
^fSpin-splitting constant $\gamma = (+)0.017$.

- (1) Bärwald, Herzberg, Herzberg, AP(Leipzig) 20, 569 (1934).
- (2) Thakur, Singh, JSRBHU 18, 253 (1967).
- (3) Chaudhry, Upadhyay, IJP 43, 83 (1969).
- (4) Wentink, Spindler, JQSRT 10, 609 (1970).
- (5) Gingerich, TA 2, 233 (1971).
- (6) Smoes, Myers, Drowart, CPL 8, 10 (1971).
- (7) Kordis, Gingerich, JCP 58, 5058 (1973).

Cr₂: ^aThermochemical value (mass-spectrom.) (1).
(1) Kant, Strauss, JCP 45, 3161 (1966).
(2) Efremov, Samoilova, Gurvich, OS(Engl. Transl.) 36, 381 (1974).

CrBr: ^aThermochemical value (flame photometry)(2).

(1) Rao, CS 18, 338 (1949).

(2) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

CrCl: ^aThermochemical value (flame photometry)(2).

(1) Rao, Rao, IJP 23, 508 (1949).

(2) See ref. (2) of CrBr.

CrCu: ^aThermochemical value (mass-spectrom.)(1).

(1) Kant, Strauss, Lin, JCP 52, 2384 (1970).

CrF: ^aThermochemical value (mass-spectrom.)(2).

^bBarrow (see DONNSPEC) points out the existence of many coincidences between band heads of system I and band heads of the $A^2\Sigma-X^2\Pi$ system of SiF.

(1) Durgavathi, Rao, IJP 28, 525 (1954).

(2) Kent, Margrave, JACS 87, 3582 (1965).

CrGe: ^aThermochemical value (mass-spectrom.)(1).

(1) Kant, Strauss, JCP 42, 3579 (1968).

Cr¹H, Cr²H:

^aDescribed as rather diffuse by (6).

^bThe weakness of the emission at low pressures, and the stronger appearance of the corresponding deuteride system suggest predissociation of the upper state through a potential hill (5).

^cSpin splitting constants $\gamma_0 = 1.20$, $\lambda_0 = 0.14$ (3)(4). Perturbations in both $v=0$ and $v=1$ may be caused by a $^8\Sigma$ state (3).

^d $H_0 = +0.7 \times 10^{-8}$; $D_1 = 2.36 \times 10^{-4}$.

^eSpin splitting constants $\gamma_0 \approx 0.1$, $\lambda_0 = 0.03$ (3)(4).

^f $H_0 = +1.0 \times 10^{-8}$; $D_1 = 3.43 \times 10^{-4}$.

(continued p.183)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(52)\text{Cr}^2\text{H}$		$(\mu = 1.93891666)$ Complex band structure in the region $27020 - 27540 \text{ cm}^{-1}$.						$B \leftrightarrow (X)$ $A \rightarrow X, \quad R \quad 11559.65 \text{ Z}$		DEC 1974 (5)(6) (4)*
B ${}^6\Pi$										
A ${}^6\Sigma(+)$	(11609)	1089	H 13	$[2.737]^g$		$[0.677]^h$	$[1.782]$			
X ${}^6\Sigma(+)$	0	(1182)		$[3.142]^i$		$[0.888]^j$	$[1.663]_5$			
$(52)\text{Cr}^{127}\text{I}$		$(\mu = 36.855845_7) \quad D_0^0 = 2.9_4 \text{ eV}^a$								DEC 1974
$(52)\text{Cr}^{14}\text{N}$		$(\mu = 11.0295312_7) \quad D_0^0 = 3.8_7 \text{ eV}^a$								DEC 1974
$(52)\text{Cr}^{16}\text{O}$		$(\mu = 12.2290254_9) \quad D_0^0 = 4.4 \text{ eV}^a$								DEC 1974
B ${}^5\Pi$	16586^b	750.5	H 9.4	$\begin{cases} 0.4874 & 0.0044 \\ 0.4801 & 0.0048 \\ 0.4751 & 0.0057 \\ 0.4735 & 0.0070 \\ 0.4675 & 0.0050 \end{cases}$			1.703	$B \rightarrow X, \quad R$	$\begin{matrix} 16487.6 & \text{H} \\ 16501.2 & \text{H} \\ 16511.3 & \text{H} \\ 16519.4 & \text{H} \\ 16515.2 & \text{H} \end{matrix}$	(1)(2)(3)* (5)* (7)
Five R shaded emission bands with multiple heads between 11800 and 11990 cm^{-1} , tentatively assigned as 1-0 sequence of a new transition by (4).										
X ${}^5\Pi$	0^c	898.4	H 6.7_5	$\begin{cases} 0.5410 & 0.0049 \\ 0.5348 & 0.0049 \\ 0.5284 & 0.0050 \\ 0.5233 & 0.0036 \\ 0.5231 & 0.0070 \end{cases}$			1.615		(11117)	(5)*
$(52)\text{Cr}^{(32)}\text{S}$		$(\mu = 19.7901878) \quad D_0^0 = 3.3_7 \text{ eV}^a$								DEC 1974
B	23448	510	H 2					$B \rightarrow A, \quad R$	23393 H	(2)
A	0	621	H 4							

Cr¹H, Cr²H (continued):

^eSpin splitting constants $\gamma_0 = 0.64$, $\lambda_0 = 0.28$. Several perturbations.

$h_{H_0} = + 0.1_0 \times 10^{-8}$.

ⁱSpin splitting constants $\gamma_0 = 0.02_3$, $\lambda_0 = 0.03$.

$j_{H_0} = + 0.07 \times 10^{-8}$.

(1) Gaydon, Pearse, Nature 140, 110 (1937).

(2) Kleman, Liljeqvist, AF 2, 345 (1955).

(3) Kleman, Uhler, CJP 37, 537 (1959).

(4) O'Connor, PRIA A 65, 95 (1967).

(5) O'Connor, JP B 2, 541 (1969).

(6) Smith, PRS A 322, 113 (1973).

CrI: ^aThermochemical value (flame photometry)(1).

(1) See ref. (2) of CrBr.

CrN: ^aThermochemical value (mass-spectrom.)(1).

(1) Srivastava, Farber, HTS 5, 489 (1973).

CrO: ^aThermochemical value (mass-spectrom.)(6).

^b|A| ≈ 100 .

^c|A| ≈ 110 . Not certain that this is the ground state.

(1) Ferguson, JRNBS 8, 381 (1932).

(2) Ghosh, ZP 78, 521 (1932).

(3) Ninomiya, JPSJ 10, 829 (1955).

(4) Gaspard, Rosen, quoted in ref. (5).

(5) Gatterer, Junkes, Salpeter, Rosen, METOX.

(6) Grimley, Burns, Inghram, JCP 34, 664 (1961).

(7) Murthy, Nagaraj, PPS 84, 827 (1964).

CrS: ^aThermochemical value (mass-spectrom.)(1).

(1) Drowart, Pattoret, Smoes, PBCS No. 8, 67, (1967).

(2) Monjazez, Mohan, SpL 6, 143 (1973).

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State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{12}\text{C}^{32}\text{S}$											
$\mu = 8.72519418$ $D_0^0 = 7.355 \text{ eV}^a$ I.P. = 11.335 eV^b											
Fragments of further band systems and Rydberg series.											
G	(81373)	[1229]						G \leftarrow X,	81347	(12)*	
F								F \leftarrow X,	77537	(12)*	
Continuous absorption to a repulsive state; $74600 - 76300 \text{ cm}^{-1}$.											
E	(71890)	[1459]	H					E \leftarrow X, (V)	71979	H (12)*	
c ($^3\Sigma^+$)								c \leftarrow X, ^c	71803	H (12)*	
C ($^1\Sigma^+$)	(71255)	[1425]	H					C \leftarrow X, ^d	71327	H (12)*	
B ($^1\Sigma^+$)	(64868)	[1332]	H					B \leftarrow X, (V)	64893	H (12)*	
A' $^1\Sigma^+$	56505	462.4	H	7.46^e	0.511_4	0.0109^f	(2.5)	1.944	A' \rightarrow X, R	56093	H (15)*
x, y		Fragments of two perturbing states ($B_x < 0.61$, $B_y < 0.77$) near 39170 and 39950 cm^{-1} .								(3)	
A new band at 39138 cm^{-1} , originally (14) attributed to a $^3\Delta$ state, is now believed to be due to $v=11$ of a $^3\Pi$ (24).											
A $^1\Pi$	38904.4	1073.4^g	Z	10.1	0.7800^{ghi}	0.0063^j	(1.65)	1.573_9	A ^k \leftrightarrow X, ^l R	38797.6	Z (1a)* (3)*
e $^3\Sigma^-$	38683	752^m		4.7	0.619_4^m	0.004_0	(1.68)	1.766	e \leftarrow X, R	38417^m	(3)*
d $^3\Delta_i^n$	35675.0	795.6^o		4.91	0.6367^o	0.0061	(1.63)	1.742_0	d \leftarrow X, R	35430.6^o	(3)* (14)(27)
a' $^3\Sigma^+$	31331.4	830.7^o		5.04	0.6489^{op}	0.0060	(1.58)	1.725_5	a' \leftarrow X, R	31104.6^o	(3)* (14)(27)
Unclassified emission bands, probably due to triplet - triplet transitions, in the region $13300 - 22200 \text{ cm}^{-1}$.											(22)*
a $^3\Pi_r$	27661.0^q	1135.1^o		7.73	0.7851^o	0.0072	$[1.9_4]^r$	1.568_7	a \rightarrow X, ^s R	27585.7^o	(8)(22)* (27)
X $^1\Sigma^+$	0	1285.08	Z	6.46	0.8200462^i	0.0059224	1.43	1.534941	Microwave sp. ^t		(1)(4)(23a)

CS, CS⁺,

^aFrom a short extrapolation of the vibrational levels in A' $1\Sigma^+$ (15), assuming that the atomic products arising at the dissociation limit are C, $3P_2$ + S, $3P_2$. The latest thermochemical (mass-spectrometric) value is 7.21 eV (18). Both values agree with an upper limit (< 7.7 eV) derived from infrared chemiluminescence studies (14a), and the corresponding heats of formation, $\Delta H_{f0}^0 = 66.11$ or 69.5 kcal/mole, respectively, are supported by photodissociation (20a) and photoionization (7a) results for CS₂. See, however, (26)(29) who suggest $\Delta H_{f0}^0 = 33$ kcal/mole, implying $D_0^0 = 8.79$ eV.

^bFrom the photoelectron spectrum (16)(17)(20).

^cSingle weak absorption band.

^dBands described as diffuse.

^e $w_e v_e = -0.108$, $w_e z_e = -0.0377$.

^f $+0.00112(v+\frac{1}{2})^2 - 0.000208(v+\frac{1}{2})^3$.

^gDeperturbed constants (3); all observed vibrational levels of this state are strongly perturbed by interactions with a 3Π , a' $3\Sigma^+$, d 3Δ , e $3\Sigma^-$ (1a)(3)(14). The following rather different set of deperturbed parameters is given by (27): $T_e = 38895.7$, $w_e = 1077.3$, $w_e x_e = 10.66$, $B_e = 0.7881$, $\alpha_e = 0.0092$.

^h Λ -doubling intervals in $v=0$ ($J=1-9$) range from 0.00045 to 0.05961 cm⁻¹ (13)(14). The variation with J of the Stark effect was observed in optical-rf double resonance and was analyzed (14) to give $\mu_{e\ell}(v=0) = 0.63$ D ($^+CS^-$); see also (13).

ⁱRKR potential functions (6).

^j $\gamma_e = -0.0004$.

^kLifetimes from Hanle effect observations $\tau(v=0) = 176$ ns (corrected for lengthening by triplet mixing), $\tau(v=2) = 203$ ns (21). The phase shift method (10) gives $\tau(v=0) = 255$, $\tau(v=1) = 339$, $\tau(v \geq 2) = 292$ ns; $f_{00} = 0.0059$.

^lMorse-potential Franck-Condon factors (5); compare with experimental values from the fluorescence spectrum excited in the VUV photolysis of CS₂ and OCS (25). C³⁴S isotopic bands (7)(11).

^mOnly $v=1$ and 2 observed (3); the vibrational numbering is from isotope studies (14). The following set of deperturbed parameters is given by (27): $T_e = 38681.9$, $w_e = 752.8$, $w_e x_e = 4.95$, $B_e = 0.6227$, $\alpha_e = 0.0062$. Spin-splitting in $v=1$: $\lambda + \frac{1}{2}\gamma = 1.75$ (3).

ⁿThis state, originally (3)(14) considered to be 3Π and labelled k, is now believed to be 3Δ (19)(24). The name has been changed to d 3Δ in order to emphasize the similarity to CO. $A \approx -50$.

^oDeperturbed constants (27).

^pSpin-splitting constant $\lambda(v=10) = -1.28$ (14).

^q $A \approx 95$ cm⁻¹.

^rFrom (22).

^sTwo subbands corresponding to $3\Pi_1 - 3\Sigma^+$ and $3\Pi_0 - 3\Sigma^+$ have been observed (22).

^tDipole moments [$^-CS^+$, see (23)] from Stark effect $\mu_{e\ell}(v=0) = 1.958$ D, $\mu_{e\ell}(v=1) = 1.936$ D (9). Zeeman effect (23), molecular g factor -0.2702. $^{32}S/^{33}S$ and $^{32}S/^{34}S$ mass ratios from microwave spectra (2).

(continued p.186)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{12}\text{C}^{32}\text{S}^+$		$D_0^0 = 6.38_0 \text{ eV}^u$								OCT 1976 A
C $2\Sigma^+$	54120	1055 ^v							53960 ^v	(20)
B $2\Sigma^+$	36470	868 ^v							36210 ^v	(20)
A $2\Pi_i$	11990 ^w	1012.8	Z 6.52	0.71776	0.00622	1.82 ^x	1.6407	A→X, R	11806.3 Z	(28)
X $2\Sigma^+$	0	1384 ^y		$[0.8640_0]^z$		$[1.26]$	$[1.4954]$			

CS, CS^+ (continued):

^u $D_0^0(\text{CS}) + \text{I.P.}(\text{S}) - \text{I.P.}(\text{CS})$.

^vFrom the photoelectron spectrum (20); see also (16).

^w $A = -298.46$ (28).

^x $\beta_e = +0.15 \times 10^{-6}$.

^yFrom the photoelectron spectrum (20); (16) and (17) give 1330 and 1290 cm^{-1} , respectively. Only one level has been found in the optical spectrum (28).

^zSpin-splitting constant $\tilde{\gamma}_0 = +0.0201$.

CS, CS⁺:

- (1) Mockler, Bird, PR 28, 1837 (1955).
- (1a) Lagerqvist, Westerlund, Wright, Barrow, AF 14, 387 (1958).
- (2) Rosenblum, Townes, Geschwind, RMP 30, 409 (1958).
- (3) Barrow, Dixon, Lagerqvist, Wright, AF 18, 543 (1960).
- (4) Kewley, Sastry, Winnewisser, Gordy, JCP 32, 2856 (1963).
- (5) Felenbok, PPS 86, 676 (1965).
- (6) Nair, Singh, Rai, JCP 43, 3570 (1965).
- (7) Narasimham, Gopal, CS 35, 485 (1966).
- (7a) Dibeler, Walker, JOSA 52, 1007 (1967).
- (8) Tewarson, Palmer, JMS 27, 246 (1968).
- (9) Winnewisser, Cook, JMS 28, 266 (1968).
- (10) Smith, JQSRT 2, 1191 (1969).
- (11) Chaudhury, Upadhyaya, Thakur, IJP 44, 375 (1970).
- (12) Donovan, Husain, Stevenson, TFS 66, 1 (1970).
- (13) Silvers, Bergeman, Klemperer, JCP 52, 4385 (1970).
- (14) Field, Bergeman, JCP 54, 2936 (1971).
- (14a) Hancock, Morley, Smith, CPL 12, 193 (1971);
Hancock, Ridley, Smith, JCS FT II 68, 2117 (1972).
- (15) Bell, Ng, Suggitt, JMS 44, 267 (1972).
- (16) Jonathan, Morris, Okuda, Smith, Ross, CPL 13, 334 (1972); FDCS No. 54, 48 (1972).
- (17) King, Kroto, Suffolk, CPL 13, 457 (1972).
- (18) Hildenbrand, CPL 15, 379 (1972).
- (19) Robbe, Schamps, CPL 15, 596 (1972).
- (20) Frost, Lee, McDowell, CPL 17, 153 (1972).
- (20a) Okabe, JCP 56, 4381 (1972).
- (21) Silvers, Chiu, JCP 56, 5663 (1972).
- (22) Taylor, Setser, Coxon, JMS 44, 108 (1972).
- (23) McGurk, Tigelaar, Rock, Norris, Flygare, JCP 58, 1420 (1973).
- (23a) Lovas, Krupenie, JPCRD 3, 245 (1974).
- (24) Bruna, Kammer, Vasudaran, CP 2, 91 (1975).
- (25) Lee, Judge, JCP 63, 2782 (1975).
- (26) Hubin-Franskin, Loch, Katihabwa, CPL 37, 488 (1976).
- (27) Cossart, Horani, Rostas, quoted by Cossart, Bergeman, JCP 65, 5462 (1976).
- (28) M. Horani, unpublished.
- (29) Hubin-Franskin, Katihabwa, Collin, IJMSIP 20, 285 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-9}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{133}\text{Cs}_2$		$\mu = 66.452718$	$D_0^0 = 0.394 \text{ eV}^a$	$3.592 < \text{I.P. (eV)}^b < 3.821$						OCT 1976 A
		Unidentified structure in the absorption spectrum from 31800 to 34900, 36700 to 41700 cm^{-1} .								(9)
		Fragments of other systems, as well as diffuse bands near atomic lines. ^c								(1)(4)
(E)		Strong system in the region 19140 - 21700, maximum at 20800 cm^{-1} .							$E^d \leftrightarrow X$,	(1)* (7)(14)
D		Weak system in the region 16500 - 18000 cm^{-1} .							$D \leftarrow X$,	(1)(7)
C ($^1\Pi_u$) 1_u	15948.60	29.703 ^e (Z)	0.0576 ^e	0.01347 ^f	0.0000785	12.10 ^g	4.34 ₀	$C^d \leftrightarrow X$, v_R 15942.45 (Z)	(1)* (2)(10)	
B ($^1\Pi_u$) 1_u	13043.88	34.329 ^h H	0.0800 ^h					$B \leftarrow X$, R 13040.03 H	(1)* (12)	
A ($^1\Sigma_u^+$)		Extended system in the region 8800 - 11500 cm^{-1} ; partial analysis.							$A \leftrightarrow X$, R	(1)(3)(8)(15)
b ($^3\Pi_u$)		Unresolved system from 8000 to 8600 cm^{-1} , maximum at 8370 cm^{-1} .							$b \leftrightarrow X$,	(8)(15)
a ($^3\Sigma_u^+$)	(3140)	Repulsive curve with small van der Waals minimum.								
X ($^1\Sigma_g^+$)	0	42.022 ⁱ	0.0823 ⁱ	0.0127 ₁ ^f	0.0000264	4.64 ^f	4.47	Mol. beam magn. reson. ^j		
$^{133}\text{Cs}_2^+$		$D_0^0 = 0.61 \text{ eV}^k$								OCT 1976
X ($^2\Sigma_g^+$)							(4.44) ^l			

Cs_2 , Cs_2^+ :

^aShort extrapolation of ground state vibrational levels (12).

^bAssociative ionization of cesium vapour (16); see also (18). (11) give an appearance potential of 3.8₀ eV, (16) recommend 3.68 eV as the most likely value.

^cSatellites and self-broadening of Cs principal lines (17) (21). Resonances in the two-photon ionization spectrum of cesium corresponding to the fundamental and diffuse series in absorption result from reactions initiated by molecular transitions to intermediate dissociative states; see (20).

^dIntermediates in the two-photon ionization of Cs_2 (19)(22).

^e w_e , ..., $w_e z_e$ obtained (10) from V shaded P heads [also observed in the magnetic rotation spectrum (12)] and calculated head-origin separations; see ^f.

^fThe rotational structure of the C-X bands is not resolved. The rotational constants for both states are based on estimated values for B_0'' , D_0'' and have been adjusted to reproduce the observed V as well as R shaded heads in the P, Q, and R branches. The red-degraded heads occur through the D terms in the rotational energy expressions. See (10).

$g_{\beta_e} = -0.193 \times 10^{-9}$; see ^f.

^h w_e , ..., $w_e z_e$ from band heads in the magnetic rotation spectrum (12). Vibrational levels up to $v'=83$ observed in absorption. The B state extrapolates to a potential maximum at $\sim 250 \text{ cm}^{-1}$ above $6^2\text{P}_{3/2} + 6^2\text{S}_{1/2}$ (12).

ⁱAverage of the constants from B-X and C-X (10)(12). Also higher order constants. Vibrational levels observed up to $v''=100$.

$j_{\text{eqQ}}(^{133}\text{Cs}) = +0.23 \text{ MHz}$ (5); $g_J = 0.00547 \mu_N$ (6).

^k $D_0^0(\text{Cs}_2) + \text{I.P.}(\text{Cs}) - \text{I.P.}(\text{Cs}_2)$; see ^b.

^lRough estimate from the analysis of charge-exchange cross sections (13). Theoretical values tend to be larger (20a).

- (1) Loomis, Kusch, PR 46, 292 (1934).
- (2) Kusch, Loomis, PR 49, 217 (1936).
- (3) Finkelburg, Hahn, PZ 39, 98 (1938).
- (4) Tsi-Ze, Shang-Yi, JPR 2, 169 (1938).
- (5) Logan, Côté, Kusch, PR 86, 280 (1952).
- (6) Brooks, Anderson, Ramsey, PRL 10, 441 (1963); PR A 136, 62 (1964).
- (7) Lapp, Harris, JQSRT 6, 169 (1966).
- (8) Bayley, Eberlin, Simpson, JCP 49, 2863 (1968).
- (9) Creek, Marr, JQSRT 8, 1431 (1968).
- (10) Kusch, Hessel, JMS 25, 205 (1968).
- (11) Foster, Leckenby, Robbins, JP B 2, 478 (1969).
- (12) Kusch, Hessel, JMS 32, 181 (1969).
- (13) Olson, PR 187, 153 (1969).
- (14) Baumgartner, Demtröder, Stock, ZP 232, 462 (1970).
- (15) Sorokin, Lankard, JCP 55, 3810 (1971).
- (16) Marr, Wherrett, JP B 5, 1735 (1972).
- (17) Niemax, PL A 38, 141 (1972).
- (18) Popescu, Pascu, Collins, Johnson, Popescu, PR A 8, 1666 (1973).
- (19) Collins, Johnson, Popescu, Musa, Pascu, Popescu, PR A 8, 2197 (1973).
- (20) Collins, Johnson, Mirza, Popescu, Popescu, PR A 10, 813 (1974).
- (20a) Bellomonte, Cavaliere, Ferrante, JCP 61, 3225 (1974).
- (21) Niemax, Pichler, JP B 7, 1204 (1974); 8, 2718 (1975).
- (22) Granneman, Klewer, Nygaard, Van der Wiel, JP B 9, 865 (1976).

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State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-9}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{133}\text{Cs}^{40}\text{Ar}$										OCT 1976 A
D								$D \rightarrow X$,		(4)
B $2\Sigma^+$								$B \leftrightarrow X$, ^b		(4) (2)(3)
A $2\Pi_{3/2}$ $2\Pi_{1/2}$								$A \leftrightarrow X$, ^b		(2)(3)
X $2\Sigma^+$										

CsAr: ^aThe bands are believed to arise from transitions between a bound Cs(7s6)-Ar excited molecular state and the unstable 6s6 ground state.

^bThe far-wing emission profiles of the collision-broadened Cs resonance lines at 11178 and 11732 cm⁻¹ have been analyzed (2) to give the potential curves for the states X, A, B in the interval 3.5-6 Å; see also the theoretical calculations of (1). Absorption coefficients in the wings of these lines have been measured (3); barely detectable maxima in the red wings may be due to vibrational structure in the A ²Π components.

(1) Baylis, JCP 51, 2665 (1969).

(2) Hedges, Drummond, Gallagher, PR A 6, 1519 (1972).

(3) Chen, Phelps, PR A 7, 470 (1973).

(4) Tam, Moe, Park, Happer, PRL 35, 85 (1975).

CsBr, CsBr⁺:

^aFrom the threshold for dissociative photoionization (13), in good agreement with the thermochemical value of (6); see also (7)(9). The value quoted here corresponds to dissociation into normal atoms; see, however, (11) who demonstrated that under some conditions (shock waves) the primary dissociation products are ions (Cs⁺ + Br⁻) rather than normal atoms in violation of the non-crossing rule.

^bPhotoionization mass-spectrometry (13). Average values (photoelectron spectroscopy) for the vertical first and second ionization potentials: 8.12 and 8.51 eV (15)(20).

^cAssociated with excitation of an electron from the metal 5p shell.

^dThe absorption and the emission bands arise from transitions between a shallow homopolar upper state (from normal atomic products) and the low- and high-lying vibrational levels, resp., of the ionic ground state.

^eDerived from the rotational constants (18). See also (5).

CsBr, CsBr⁺ (continued):

$$f + 1.02 \times 10^{-7} (v + \frac{1}{2})^2 + 3.2 \times 10^{-10} (v + \frac{1}{2})^3 \quad (18).$$

$$E\beta_e = +0.0064 \times 10^{-9}; \text{ also higher order constants (18).}$$

$$h_{\text{rel}} = 10.82 \text{ D (molecular beam electric deflection) (21);}$$

$$\text{eqQ}({}^{79}\text{Br}) = -[6.79 - 0.73(v + \frac{1}{2})] \text{ MHz (14);}$$

$$g_J(v=0) = (-)0.009 \mu_N \quad (16).$$

ⁱFrom I.P.(CsBr) and the threshold energy for dissociative ionization (Cs⁺ from CsBr), see (13). (20) give 0.24 eV.

^jFrom the photoelectron spectrum (15)(20). The two observed broad peaks (see ^b) correspond to removal of an electron from the halogen 4p shell.

(1) Müller, AP(Leipzig) 82, 39 (1927).

(2) Sommermeyer, ZP 56, 548 (1929).

(3) Barrow, Caunt, PRS A 219, 120 (1953).

(4) Honig, Stitch, Mandel, PR 92, 901 (1953);

Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).

(5) Rice, Klemperer, JCP 27, 573 (1957).

(6) Brewer, Brackett, CREV 61, 425 (1961).

(7) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(8) Rusk, Gordy, PR 127, 817 (1962).

(9) Scheer, Fine, JCP 36, 1647 (1962).

(10) Davidovits, Brodhead, JCP 46, 2968 (1967).

(11) Berry, Cernoch, Coplan, Ewing, JCP 49, 127 (1968).

(12) Geiger, Pfeiffer, ZP 208, 105 (1968).

(13) Berkowitz, JCP 50, 3503 (1969).

(14) Hoelt, Tiemann, Törring, ZN 27 a, 702 (1972).

(15) Berkowitz, Dehmer, Walker, JCP 59, 3645 (1973).

(16) Honerjäger, Tischer, ZN 28 a, 458 (1973).

(17) Miller, Finney, Inman, AD 5, 1 (1973).

(18) Honerjäger, Tischer, ZN 29 a, 819 (1974).

(19) Oldenborg, Gole, Zare, JCP 60, 4032 (1974).

(20) Potts, Williams, Price, PRS A 341, 147 (1974).

(21) Story, Hebert, JCP 64, 855 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{133}\text{Cs}^{35}\text{Cl}$											
		$\mu = 27.6847083$		$D_0^0 = 4.58 \text{ eV}^a$		$\text{I.P.} = 8.3_2 \text{ eV}^b$				NOV 1976 A	
		Strong autoionization peaks ^c at and above 12.4 eV in photoionization (15) and electron energy loss spectra (13).								(13)(15)	
		Absorption continua with maxima at 51500 and 40500 cm^{-1} (1)(3)(12), followed by diffuse absorption bands (fluctuation b.) from 40850 to 29840 cm^{-1} (3). The chemiluminescence spectrum (21) consists of a long lower-state vibrational progression and extends from 29400 to 20800 cm^{-1} . See ^d of CsBr.								(1)(3)(12) (21)	
X $1\Sigma^+$	0	214.17 ^d	0.731 ^d	0.07209149	0.00033756 ^e	0.32675 ^f	2.90627 ₂	{ IR sp. Microwave sp. ^g Mol. beam el. reson. ^h Mol. beam magn. reson.		(6) (4)(10)(19) (20) (2)(5)(14) (11)	
$^{12}\text{C}^{80}\text{Se}$											
A 1Π	(35243)	$\mu = 10.43336114$		$D_0^0 = 5.9_8 \text{ eV}^a$			$[1.82_1]$		A \leftrightarrow X, R 35135.25 ^d	NOV 1976	
		$[817.7]^b$		$[0.487]^c$						(1)* (2)(3)* (6)*	
		(not observed)									
a 3Π	$\begin{cases} 2 \\ 1 \\ 0^+ \end{cases}$	(24466)		$[0.544]$			$[1.72_3]$	a \rightarrow X, R 24396.6 Z	(4)		
		(24150)		$[0.544]$				24080.0 Z			
X $1\Sigma^+$	0	1035.36	Z 4.86	0.5750 ^e	0.00379	7.1 ^f	1.67647 ^g	Microwave sp. ^h	(5)		

CsCl: ^aThermochemical value (7), confirmed by the photoionization data of (15). See also (8)(9).

^bOnset of a broad band in the photoelectron spectrum, maximum (vertical I.P.) at 8.75 eV (22). The photoelectron spectrum was also investigated by (17) who find 7.84 and 8.54 eV, respectively.

CsCl (continued):

^cInterpretation analogous to CsBr (footnote ^c).

^dCalculated from the rotational constants (20). Good agreement with the less precise values from the infrared spectrum (6).

^e $+ 3.42 \times 10^{-7}(v+\frac{1}{2})^2 + 1.8 \times 10^{-9}(v+\frac{1}{2})^3$ (20).

CsCl (continued):

- $f/\beta_e = + 0.00038 \times 10^{-7}$; also higher order constants (20).
 $\epsilon_{eqQ}(^{35}\text{Cl}) = + [1.830 - 0.118(v+\frac{1}{2})]$ MHz,
 $|\epsilon_{eqQ}(^{133}\text{Cs})| \leq 1.1$ MHz (16).
 $g_J = - [0.02815 - 0.00031(v+\frac{1}{2})] \mu_N$ (18); see, however, (11) who give $g_J = (-)0.0212$.
 $h\mu_{el} = [10.358 + 0.058(v+\frac{1}{2})]$ D (14).
 (1) Schmidt-Ott, ZP 69, 724 (1931).
 (2) Luce, Trischka, PR 82, 323; 83, 851 (1951); JCP 21, 105 (1953).
 (3) See ref. (3) of CsBr.
 (4) See ref. (4) of CsBr.
 (5) Trischka, JCP 25, 784 (1956).
 (6) See ref. (5) of CsBr.
 (7) See ref. (6) of CsBr.
 (8) See ref. (7) of CsBr.
 (9) See ref. (9) of CsBr.
 (10) Clouser, Gordy, PR A 134, 863 (1964).
 (11) Mehran, Brooks, Ramsey, PR 141, 93 (1966).
 (12) See ref. (10) of CsBr.
 (13) See ref. (12) of CsBr.
 (14) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
 (15) See ref. (13) of CsBr.
 (16) Hoeft, Tiemann, Törring, ZN 27 a, 1516 (1972).
 (17) See ref. (15) of CsBr.
 (18) See ref. (16) of CsBr.
 (19) See ref. (17) of CsBr.
 (20) See ref. (18) of CsBr.
 (21) See ref. (19) of CsBr.
 (22) See ref. (20) of CsBr.

CSe: ^aThermochemical value (mass-spectrom.)(3a).

^b $\Delta G(3/2) = 833.7$; from the Q(1) lines of the 0-1, 1-1, 2-1 bands (6). This state is strongly perturbed and no meaningful vibrational and rotational constants can be given. The absorption spectrogram of (3) shows in addition to $^1\Pi - ^1\Sigma$ some absorption bands probably due to some of the perturbing levels, in particular one progression which may be a $^3\Sigma^+ \leftarrow X^1\Sigma^+$ in analogy to CO and CS.

^c $B_1 = 0.497$, $B_2 = 0.482$, $B_3 = 0.447$; see ^b.

^dQ(1) line for the 0-0 band (6).

^e $B_0 = 0.573155$ from the microwave spectrum (5).

^f $\beta_e = - 0.25 \times 10^{-7}$.

^gFrom the B_0 values for various isotopes obtained from the microwave spectrum (5).

^hDipole moment from Stark effect 1.99 D (5); molecular g factor from Zeeman effect -0.2431.

- (1) Barrow, PPS 51, 989 (1939).
 (2) Laird, Barrow, PPS 66, 836 (1953).
 (3) Callear, Tyerman, TFS 61, 2395 (1965).
 (3a) D. Detry (unpublished), quoted in DONNSPEC (1970).
 (4) Lebreton, Bosser, Marsigny, JP B 6, L226 (1973).
 (5) McGurk, Tigelaar, Rock, Norris, Flygare, JCP 58, 1420 (1973).
 (6) Stringat, Bacci, Pischedda, CJP 52, 813 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{133}\text{Cs}^{19}\text{F}$		$\mu = 16.6223003$	$D_0^0 = 5.1_5 \text{ eV}^a$	$\text{I.P.} = 8.8_0 \text{ eV}^b$						NOV 1976
		Several autoionizing states ^c at and above 12.1 eV (16), also observed in the electron energy loss spectra of (14).								(14)(16)
		Continuous absorption with maximum at 47700 cm^{-1} , preceded by diffuse absorption bands (fluctuation b.) in the region $43700 - 36900 \text{ cm}^{-1}$. See ^d of CsBr.								(2)
X $1\Sigma^+$	0	352.56^d	1.61_5^d	0.18436969	0.0011756_2^e	0.20168^f	2.345351	IR sp.		(12)
								Microwave sp.	(3)	(10)(20)(21)
								Mol. beam el. reson. ^g		(1)(4)(9)
								Mol. beam magn. reson.		(13)(15)(17)
										(11)
$^{133}\text{Cs}^1\text{H}$		$\mu = 1.00024037$	$D_0^0 = 1.81 \text{ eV}^a$							NOV 1976
a ($^3\Delta$)	$[28534]^b$	$[276]^b$	$[1.51]^b$							(4)
B $1\Sigma^+$	$[28350.5]^c$	$[82.1]^c$ Z	$[0.70]^c$					(4.63)	$B \leftarrow X, \quad R \quad 27908.2^c \quad Z$	(4)
A $1\Sigma^+$	17845.8	165.7 Z -7.7_7^d	1.075	-0.021_9^e	98^f	3.96_0		$A \leftrightarrow X, \quad R \quad 17488.3 \quad Z$		(1)(2)(5)
X $1\Sigma^+$	0	891.0 Z 12.9_3^g	2.7099	0.0579	$[113]$	2.4938				
$^{133}\text{Cs}^2\text{H}$		$\mu = 1.98403535$								NOV 1976
A $1\Sigma^+$	(17833)	(123.9) $(-3.08)^h$	i						$A \leftarrow X, \quad R \quad j$	(2)(3)
X $1\Sigma^+$	0	$[619.1]$ H	$[1.354]$	$[20]$				$[2.505]$		
$^{133}\text{Cs}^4\text{He}$		$\mu = 3.8855843_3$								NOV 1976 A
Potential curves for X $^2\Sigma$, A $^2\Pi$, and B $^2\Sigma$ in the interval $r = 3.5$ to 5.5 \AA have been derived from the analysis of the extreme-wing emission profiles of the Cs resonance lines at 11178 and 11732 cm^{-1} . Only A $^2\Pi_{3/2}$ has a small potential minimum, $D_e \approx 170 \text{ cm}^{-1}$.										(1)

CsF: ^aThermochemical value (5); see also (6)(7)(18).

^bAdiabatic ionization potential from the photoelectron spectrum (19); vertical I.P. at 9.6₀ eV.

^cInterpretation analogous to CsBr (footnote ^c).

^dDerived from the rotational constants (21); good agreement with infrared results (12). See also (8).

^e $+ 1.18 \times 10^{-6}(v+\frac{1}{2})^2 + 1.77 \times 10^{-8}(v+\frac{1}{2})^3$ (21).

^f $\beta_e = + 0.00031 \times 10^{-6}$; also higher order constants (21).

^g $\mu_{el} = [7.8478 + 0.07026(v+\frac{1}{2}) + 0.000195(v+\frac{1}{2})^2]$ D (15)(17);

$eqQ(^{133}\text{Cs}) = + [1245.2 - 16.2(v+\frac{1}{2}) + 0.31(v+\frac{1}{2})^2]$ kHz (13)(17);

$g_J(v=0) = (-)0.06420 \mu_N$, for $v \neq 0$ see (9)(20); see also (11).

(1) Trischka, PR 74, 718 (1948); 76, 1365 (1949).

(2) See ref. (3) of CsBr.

(3) See ref. (4) of CsBr.

(4) See ref. (5) of CsCl.

(5) See ref. (6) of CsBr.

(6) See ref. (7) of CsBr.

(7) See ref. (9) of CsBr.

(8) Ritchie, Lew, CJP 42, 43 (1964).

(9) Gräff, Runolfsson, ZP 187, 140 (1965).

(10) Veazey, Gordy, PR A 138, 1303 (1965).

(11) See ref. (11) of CsCl.

(12) Baikov, Vasilevskii, OS(Engl. Transl.) 22, 198 (1967).

(13) English, Zorn, JCP 47, 3896 (1967).

(14) See ref. (12) of CsBr.

(15) See ref. (14) of CsCl.

(16) See ref. (13) of CsBr.

(17) Bennowitz, Haerten, Klais, Müller, CPL 9, 19 (1971);
ZP 242, 168 (1971).

(18) JANAF (1971).

(19) See ref. (15) of CsBr.

(20) See ref. (16) of CsBr.

(21) See ref. (18) of CsBr.

Cs¹H, Cs²H:

^aShort extrapolation of vibrational levels in B ¹ Σ^+ to the limit ²D + ²S (4). A longer extrapolation of the ground state levels (5) gives 2.08 eV.

^bConstants for the lowest of three levels observed in small perturbations of B ¹ Σ^+ ; A ≈ 14 . Vibrational numbering unknown, $\Omega = 3$ not observed.

^cConstants for the lowest of eleven observed levels, $v' = 11 \pm 3$. ΔG increases to 93.7 for $v=18$; $B_v(v \leq 18) = 0.787 - 0.0076(v+\frac{1}{2})$. For $v > 18$ both ΔG and B_v decrease rapidly.

^d $- 0.297(v+\frac{1}{2})^3 + 0.0040(v+\frac{1}{2})^4$ (valid for $v \leq 15$).

^e $- 0.00131(v+\frac{1}{2})^2$ (valid for $v \leq 13$).

^f $\beta_e = - 2.0 \times 10^{-6}$.

^g $w_{ey_e} = + 0.105$, $w_{ez_e} = - 0.0018$. Observed up to $v''=14$ in laser-excited fluorescence (5).

^h $w_{ey_e} = - (0.058)$; from band heads, $8 \leq v' \leq 18$.

ⁱOnly the 10-0 and 11-0 bands have been rotationally analyzed (2); $B_{10} = 0.587$, $B_{11} = 0.586$.

^jBand origins for the 10-0 and 11-0 bands at 19091.2 and 19261.8 cm^{-1} .

(1) Almy, Rassweiler, PR 53, 890 (1938).

(2) Bartky, JMS 21, 25 (1966).

(3) Császár, Koczka, APH 23, 211 (1967).

(4) Ringström, JMS 36, 232 (1970).

(5) Tam, Happer, JCP 64, 2456 (1976).

CsHe: (1) See ref. (2) of CsAr.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{133}\text{Cs}(^{20}\text{Ne})$		$(\mu = 17.3782925)$ Strong emission at 18020 and a narrow band at 18570 cm^{-1} , as well as weaker bands in the $14000 - 15000\text{ cm}^{-1}$ region; see the analogous transitions of CsAr and CsKr. The molecular states associated with the Cs resonance lines at 11178 and 11732 cm^{-1} (see Cs-Ar, He, Kr) are unstable except $A\ ^2\Pi_{3/2}$ which has a potential minimum of $\sim 130\text{ cm}^{-1}$.								NOV 1976 A (2) (1)

CsI, CsI^+ :

- ^aAverage of a thermochemical value (6) and a value obtained from photodissociative ionization of CsI (12). See also (7)(9).
- ^bFrom photoionization mass-spectrometry (12). The adiabatic ionization potential from photoelectron spectroscopy (14)(18) is 7.10 eV; the first and second vertical potentials are 7.54 and 8.46 eV (average values).
- ^cDerived from the rotational constants (16). See also (3)(5).
- ^d $+4.89 \times 10^{-8}(v+\frac{1}{2})^2 + 1.14 \times 10^{-10}(v+\frac{1}{2})^3$ (16).
- ^e $\beta_e = +0.0023_0 \times 10^{-9}$; also higher order constants (16).
- ^f $\mu_{el} = 11.6_9\text{ D}$ (molecular beam electric deflection)(19);
 $\text{eqQ}(^{127}\text{I}) = -[14.28 + 2.10(v+\frac{1}{2})]\text{ MHz}$,
 $|\text{eqQ}(^{133}\text{Cs})| \leq 1\text{ MHz}$ (13);
 $|g_J| < 0.0036\ \mu_N$ (15).
- ^gFrom the photoionization data of (12). Using 7.10 instead of 7.25 eV for I.P.(CsI) (see ^b) would increase this value to 0.36 eV.

CsI, CsI^+ (continued):

- (1) See ref. (2) of CsBr.
 (2) See ref. (1) of CsCl.
 (3)
 \vdots See ref. (3)...(10) of CsBr, respectively.
 (10)
 (11) See ref. (12) of CsBr.
 (12) See ref. (13) of CsBr.
 (13) Hoeft, Tiemann, Törring, ZN 27 a, 1017 (1972).
 (14) See ref. (15) of CsBr.
 (15) See ref. (16) of CsBr.
 (16) See ref. (18) of CsBr.
 (17) See ref. (19) of CsBr.
 (18) See ref. (20) of CsBr.
 (19) See ref. (21) of CsBr.

CsKr, CsNe:

- (1) See ref. (2) of CsAr.
 (2) See ref. (4) of CsAr.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{133}\text{Cs}^{16}\text{O}$ X $^2\Sigma^+$ 0		$\mu = 14.2767370_3$ Ground state symmetry from matrix ESR spectroscopy (2) and magnetic and electric deflection analysis of Cs + NO ₂ scattering products (1).								NOV 1976 (1)(2)
$^{133}\text{Cs}^{(132)}\text{Xe}$		$(\mu = 66.201451_7)$ Absorption bands arising from molecular upper states correlated with various excited levels of atomic Cs, 22100 - 24700 cm^{-1} . Strong emission at 17470, accompanied by much weaker features at 18500 cm^{-1} (3); also observed in absorption (4). The blue wing of the main peak shows undulations which may be due to vibrational levels in the upper state. See the analogous transitions of Cs-Ar, Kr, Ne. Complex structure in emission and absorption from 13500 to 15900 cm^{-1} ; see Cs-Ar, Kr, Ne. The analysis of the far-wing emission profiles of the Cs resonance lines at 11178 and 11732 cm^{-1} [(2); see also (1)] shows that B $^2\Sigma$ is unstable, A $^2\Pi_{\frac{1}{2}}$ and $^2\Pi_{\frac{3}{2}}$ have potential minima of 430 and 500 cm^{-1} , resp., and X $^2\Sigma$ is very weakly bound.								NOV 1976 A (4) (3)(4)(5) (3)(4)(5) (2)
$^{63}\text{Cu}_2$		$\mu = 31.464794_9$ Additional band systems attributed to Cu ₂ in the regions 34500 - 37000, 39000 - 40100, and 40600 - 42900 cm^{-1} . No analysis.	$D_0^0 = 2.03 \text{ eV}^a$			I.P. = 7.37 eV^b				DEC 1974 A (5)
B $^1\Sigma_u^+$	21758.35	[242.15] Z	2.0 ^c H	0.09889 ₀	0.000606	6.30	2.3276	B \leftrightarrow X, R 21747.88 Z		(1)* (2)(7) (8)(10)
A ($^1\Pi_u$)	20433.2	191.9 H	0.348 ^d	(0.08185)	(0.00062)	(3.8)	(2.558 ₄)	A \leftrightarrow X, R 20396.0 H		(1)* (2)(7) (9)
X $^1\Sigma_g^+$	0	[264.55] Z	1.025 ^e H	0.10874 ₃	0.000614	7.16	2.2197			

- CsO: (1) Herm, Herschbach, JCP 52, 5783 (1970).
 (2) Lindsay, Herschbach, Kwiram, JCP 60, 315 (1974).
- CsXe: (1) Herman, Herman, JQSRT 4, 487 (1964).
 (2) Hedges, Drummond, Gallagher, PR A 6, 1519 (1972).
 (3) Tam, Moe, Park, Happer, PRL 35, 85 (1975).
 (4) Happer, Moe, Tam, PL A 54, 405 (1975).
 (5) Sayer, Ferray, Lozingot, Berlande, JP B 2, L293 (1976).

- Cu₂: ^aThermochemical value (mass-spectrom.)(3)(4)(6), re-calculated (12).
^bExperimental value by (11), quoted in an ab initio study of Cu₂ and Cu₂⁺ by (13). No details.
^c $w_e v_e = -0.02$.
^d $w_e v_e = -0.018$.
^e $w_e v_e = +0.0008$.
- (1) Kleman, Lindkvist, AF 8, 333 (1954).
 (2) Ruamps, CR 238, 1489 (1954).
 (3) Drowart, Honig, JCP 25, 581 (1956); JPC 61, 980 (1957).
 (4) Schissel, JCP 26, 1276 (1957).
 (5) Ruamps, AP(Paris) 4, 1111 (1959).
 (6) Ackerman, Stafford, Drowart, JCP 33, 1784 (1960).
 (7) Åslund, Barrow, Richards, Travis, AF 30, 171 (1965).
 (8) Pesič, Weniger, CR B 272, 46 (1971).
 (9) Pesič, Weniger, CR B 273, 602 (1971).
 (10) Rao, Lakshman, JQSRT 11, 1157 (1971).
 (11) Cabaud, Ph.D. Thesis (U. Claude Bernard, Lyon, 1972).
 (12) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).
 (13) Joyes, Leleyter, JP B 6, 150 (1973).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{63}\text{Cu}^{27}\text{Al})$		$(\mu = 18.8846172) \quad D_0^0 = 2.2_1 \text{ eV}^a$								DEC 1974
$(^{63}\text{Cu}^{75}\text{As})$		$(\mu = 34.201994_0)$ Sequences of mostly V shaded bands in thermal emission at 13529, 13531, 14134, 14633, 14684, 14811 cm^{-1} . $w' < w''$.								DEC 1974 (1)
$^{63}\text{Cu}^{209}\text{Bi}$		$\mu = 48.365456_8$								DEC 1974
B	$x_2 + 19708.6$	197.4	H	0.62				B \rightarrow X ₂ , R	19708.0 H	(1)* (2)
A	15922.0	196.9	H	0.85				A \rightarrow X ₁ , V _R	15920.6 H	(1)(2)
X ₂	x_2	198.6	H	0.55						
X ₁	0	199.6	H	0.66						
$^{63}\text{Cu}^{79}\text{Br}$		$\mu = 35.011427_7 \quad D_0^0 = 3.4_3 \text{ eV}^a$								NOV 1975
D ($^1\Sigma^+$)	25538.6	281.9	H	1.35				D \rightarrow X, R	25522.1 H	(3)*
C ($^1\Sigma^+ (0^+)$)	23460.9	294.7 ^b	Z	1.06	0.0942 ^b	0.0004 ₁	3	C \leftrightarrow X, R	23450.9 Z	(1)(4)*
B ($^1\Pi$)	23044.7	284.22	H	1.32				B \leftrightarrow X, ^c R	23029.3 H	(1)
A ($^1\Pi$)	20498.5	296.13	H	1.01				A \leftrightarrow X, ^c R	20489.2 H	(1)
X	$^1\Sigma^+$	0	314.8 ^b	Z	0.96	0.10192625	0.00045214 ^d	4.2737 ^e	2.17344 ₁ ^f	Microwave sp. (5)

CuAl: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1) Blue, Gingerich, 16th Annual Conference on Mass Spectrometry and Allied Topics, Pittsburgh (May 1968); paper 129.
- (2) Uy, Drowart, TFS 67, 1293 (1971).

CuAs: (1) Lefebvre, Houdart, CR B 274, 178 (1972).

CuBi: ^aFor rotational constants derived from incompletely resolved rotational structure in the 0-0 bands see (2). Uncertain.

^bIt is not known whether X_1 is the ground state, nor is it clear whether or not X_1 and X_2 are identical.

- (1) Lefebvre, Houdart, CR B 270, 1485 (1970); 272, 1301 (1971).
- (2) Lefebvre, Bocquet, Houdart, RPA 8, 149 (1973).

CuBr: ^aThermochemical value (2).

^bVibrational and rotational constants derived from data for the C-X system of $^{63}\text{Cu}^{81}\text{Br}$ [Tables II and III of (4)] using $\mu_i/\mu = 1.01108$.

^cThese bands appear to have R and Q heads (3).

$$d + 6.78 \times 10^{-7}(v + \frac{1}{2})^2 - 1.0 \times 10^{-9}(v + \frac{1}{2})^3.$$

$$^e\beta_e = -0.00187 \times 10^{-8}; H_e = -5.074 \times 10^{-15}.$$

^fFrom the corrected $B_e = 0.1019274$.

- (1) Ritschl, ZP 42, 172 (1927).
- (2) Brewer, Lofgren, JACS 72, 3038 (1950).
- (3) Rao, Apparao, PIAS A 60, 57 (1964).
- (4) Rao, Apparao, CJP 45, 2805 (1967).
- (5) Manson, De Lucia, Gordy, JCP 63, 2724 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{65}\text{Cu}^{35}\text{Cl}$		$\mu = 22.7279945$ $D_0^0 = 3.93 \text{ eV}^a$								DEC 1975
F $^1\Pi$ (1)	25285.30	384.94	Z	1.65	0.1607	0.00091	1.2	2.148	$F \leftrightarrow X$, R 25270.11 Z	(2)(4)(5)* (7)* (11)
E $^1\Sigma^+(0^+)$	23074.24	403.30	Z	1.62 ^b	0.1663	0.00108	1.0	2.112	$E \leftrightarrow X$, R 23068.23 Z	(1)(3)(4)(5) (9)* (11)
D $^1\Pi$ (1)	22969.74	392.89	Z	1.74 ₅	0.1677₇^c	0.0009₈		2.102 ₆	$D \leftrightarrow X$, R 22958.50 Z	(1)(4)(5) (9)* (11) (15)
C $^1\Sigma^+(0^+)$	20630.94	396.93	Z	1.48 ^d	0.1691 ^e	0.00089	1.2	2.094	$C \leftrightarrow X$, R 20621.78 Z	(1)(4)(5)(6) (8)*
B $^1\Pi$ (1)	20484.08	399.29	Z	1.61 ^d	0.1684^f_e	0.00092	1.2	2.099	$B \leftrightarrow X$, R 20476.07 Z	(1)(4)(5)(6) (8)*
A $^1\Pi$ (1)	19001.4	407.0	H	1.70					$A \leftrightarrow X$, R 18997.2 H	(1)(5)*
A' ($^1\Sigma^+$)	(13440)	(510) ^g							(A' \rightarrow X), V 13479.5 H	(13)
X $^1\Sigma^+$	0	415.29 ^e	Z	1.58	0.17628802 ^h	0.00099647 ⁱ	1.2706 ₀ ^j	2.051183 ^k	Microwave sp.	(14)
$^{63}\text{Cu}^{19}\text{F}$		$\mu = 14.5928363$ $D_0^0 = 4.4_2 \text{ eV}^a$								AUG 1975
C $^1\Pi$	20258.4 ₇	645.0 ₇	H ^Q	4.19	[0.3746] ^b		(5.1)	[1.756 ₁]	$C \leftrightarrow X$, R 20269.62 Z	(1)(2)*
B $^1\Sigma^+$	19717.5	657.0	c	3.9 ₂	0.3716	0.0032 ^d	(4.8)	1.763 ₂	$B \leftrightarrow X$, R 19734.66 Z	(1)(2)*
A $^1\Pi$	17543.4	649.2 ^e	H ^Q	4.0 ₀	[0.3675] ^f			[1.773 ₀]	$A \leftrightarrow X$, R 17556.7 H ^Q	(1)(2)
X $^1\Sigma^+$	0	622.6 ₅	H ^Q	3.95	0.3794029	0.0032298 ^g	5.63	1.744930	Microwave sp. ^h	(5)(6)
$^{(63)}\text{Cu}^{(69)}\text{Ga}$		$(\mu = 32.895626_8)$								DEC 1974
A	15276.7	151.1	H	2.28					$A \rightarrow X$, R 15240.8 H	(1)
X	0	222.0	H	0.55						
$^{(63)}\text{Cu}^{(74)}\text{Ge}$		$(\mu = 33.991986_3)$ $D_0^0 = 2.0_9 \text{ eV}^a$								DEC 1974

CuCl : ^aThermochemical value (mass-spectrom.)(10)(12).
^b $w_e y_e = -0.009_3$ (recalculated for $v \leq 4$).
^c Λ -type doubling $\Delta v_{ef}(v=0) = -0.0011_1 J(J+1)$.
^dFrom the value for the $^{63}\text{Cu}^{35}\text{Cl}$ isotope [see (6)].
^eConsistent with constants for $^{63}\text{Cu}^{35}\text{Cl}$ in (6).
^f Λ -type doubling $\Delta v_{ef}(v=0) = -0.0008_7 J(J+1)$.
^gPreliminary data.
^hFor constants of $^{63}\text{Cu}^{35}\text{Cl}$, $^{63}\text{Cu}^{37}\text{Cl}$, $^{65}\text{Cu}^{37}\text{Cl}$ see (14).
ⁱ $+1.96_4 \times 10^{-6}(v+\frac{1}{2})^2 - 2 \times 10^{-9}(v+\frac{1}{2})^3$.
^j $\beta_e = -0.0007_6 \times 10^{-7}$; $H_e = -2.007 \times 10^{-14}$.
^kFrom the corrected $B_e = 0.1762895 \text{ cm}^{-1}$ [see (14)].

- (1) Ritschl, ZP 42, 172 (1927).
- (2) Bloomenthal, PR 54, 497 (1938).
- (3) Sinha, CS 17, 208 (1948).
- (4) Asundi, Rao, Brody, Nature 192, 444 (1961).
- (5) Rao, Brody, JCP 35, 776 (1961).
- (6) Lagerqvist, Lazarova-Girsamof, Naturw. 48, 68 (1961); AF 20, 543 (1962).
- (7) Rao, Asundi, Brody, CJP 40, 412 (1962).
- (8) Rao, Asundi, Brody, CJP 40, 423 (1962).
- (9) Rao, Brody, Asundi, CJP 40, 1443 (1962).
- (10) Hildenbrand, JCP 52, 5751 (1970).
- (11) Puri, Mohan, IJPAP 8, 759 (1970); CS 43, 340 (1974).
- (12) Guido, Gigli, Balducci, JCP 57, 3731 (1972).
- (13) Rao, Rao, SpL 7, 463 (1974).
- (14) Manson, De Lucia, Gordy, JCP 62, 1040 (1975).
- (15) Ahmed, Barrow, JP B 8, L362 (1975).

CuF : ^aThermochemical value (mass-spectrom.)(4). See also (3).
^b Λ -type doubling $\Delta v_{ef} = +0.0010 J(J+1)$.
^cFrom bandheads, taking into account head-origin separations.
^dSlight modification of the analysis of the 1-1 band in (2).
^e0-0 sequence only. Constants recalculated assuming that the lower state is $X^1\Sigma^+$.
^fFrom a partial rotational analysis, assuming that the lower state is $X^1\Sigma^+$.
^g $r_e = +0.0000123$.
^h $\mu_{el}(v=0) = 5.7_7$ D. Values for $eqQ(\text{Cu})$ in (5), magnetic constants from Zeeman effect measurements in (6).

- (1) See ref. (1) of CuCl .
- (2) Woods, PR 64, 259 (1943).
- (3) Kent, McDonald, Margrave, JPC 70, 874 (1966).
- (4) Hildenbrand, JCP 48, 2457 (1968).
- (5) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 35 (1970).
- (6) Honerjäger, Tischer, ZN 29 a, 1919 (1974).

CuGa : (1) Biron, CR B 271, 1096 (1970).

CuGe : ^aThermochemical value (mass-spectrom.)(1).
 (1) Kant, Strauss, JCP 49, 3579 (1968).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{63}\text{Cu}^1\text{H}$										
		$\mu = 0.99193919$	$D_0^0 = 2.7_3 \text{ eV}^a$						JAN 1975	
D $^1\Pi$	(44669)	[1804.0]	Z (55)	7.72 ^b	0.31	4.76 ^c	1.484	D \leftarrow X, R	44651.2 Z	(2)*
d $^3\Pi_r$	(41000) ^{de}	[1760] ^e		[7.8] ^e		[10] ^e	[1.48]		40920 ^{fe}	(10)
E $^1\Sigma^+$	39299	574 ^g	Z - 3.6 ^h	3.09 ^g	- 0.03 ^h	3.8 ^h	2.34 ₄	E \leftarrow X, R	38626 ^g	(10)
b Δ_2	(28470)	[(1475)] ⁱ		[(6.7)] ^j			[(1.59)]	b \leftarrow X, R	(28250) ⁱ	(9)
e ($^3\Pi_2$) 2				[>6.2] ^j			[<1.65]		>27958 ^{fj}	(9)
c 1	(28161)	[1388.7]	Z (85)	6.43 ^k	0.42		1.626	c \leftrightarrow X, R	27957.5 Z	(3)(4)(9)
C 1	27270.4	1627.3	Z 86.0 ^l	6.55 ^m	0.352 ⁿ	[4.76] ⁿ	1.610 ₄	C \leftrightarrow X, R	27101.3 Z	(3)(4)(9)*
a ($^3\Sigma^+$)				[(5.9)] ^o					(26365) ^{fo}	(4)(9)
B $^3\Pi_0^+$	26420.9	1669.7 ^p	Z 51.2	6.582	0.290 ^p	[4.05] ^p	1.606 ₉	B \leftrightarrow X, R	26281.7 Z	(1)(4)(9)
A $^1\Sigma^+$	23434.2	1698.4	Z 44.0 ^q	6.874 ^r	0.263 ^q	4.35 ^{eq}	1.572 ₄	A \leftrightarrow X, R	23311.1 Z	(1)(4)(8)(9)
X $^1\Sigma^+$	0	1941.26	Z 37.51 ^t	7.9441	0.2563 ^t	5.20 ^t	1.46263			
$^{63}\text{Cu}^2\text{H}$										
		$\mu = 1.95163876$	$D_0^0 = 2.7_6 \text{ eV}^a$						JAN 1975	
c 1		b		[3.1614] ^c	b	[0.73] ^{db}	[1.6529 ₅]	c \leftarrow X, R	27989.11 Z	(3)
C 1	27271.6	1143.5	Z 29.9	[3.2589] ^e	0.131	[1.211] ^e	1.611 ₉	C \leftarrow X, R	27148.59 ^{ez}	(3)
a $^3\Sigma^+$	(26490)	[(1090)] ^f		[3.20] ^f	0.10		1.63 ₀	a \leftarrow X, R	(26346) ^f	(3)
B $^3\Pi_0^+$	26381.8	1222.0	Z 35.7	3.317 ^g	0.086	[1.2] ^g	1.613 ₇	B \leftarrow X, R	26296.5 Z	(3)
A $^1\Sigma^+$	23412.9	1210.9	Z 19.50 ^h	3.521	0.096 ⁱ	[1.16] ^j	1.566 ₃	A \leftrightarrow X, R	23326.1 Z	(1)(2)(3)
X $^1\Sigma^+$	0	1384.14	Z 18.97	4.0381	0.0917	[1.362] ^k	1.4625 ₅			

Cu^1H : ^aExtrapol. of A $^1\Sigma^+$ to the limit $\text{Cu}(^2D_{5/2}) + \text{H}(^2S)$. Predissociation in A $^1\Sigma^+$ gives <2.89 eV, flame photom. (?) 2.86 eV.
^b Λ -type doubling $\Delta v_{ef} = +0.047 J(J+1)$, for $J < 15$.
^c $\beta_e = +0.68 \times 10^{-4}$.
^d $A \approx +117$.
^eFrom perturbations in E $^1\Sigma^+$; vibr. numbering uncertain.
^f T_0 , referring to X $^1\Sigma^+(v=0)$.

Cu^1H (continued):

^gLowest observed level is $v=3$. Numerous perturbations in $v=4\dots 11$ by three levels of d $^3\Pi_r$.
 $h_{we} y_e = -0.27$; $y_e = -0.0048$; $\beta_e = -0.08 \times 10^{-4}$.
ⁱ $v=0,1$ interact with $v=1,2$, resp., of C 1. Deperturbed constants for $v=1$ (e levels) are $B = 6.36_4$, $D = 7.6 \times 10^{-4}$.
^jFrom a perturbation in $v=0$ of c 1.

Cu¹H (continued):

^kDeperturbed constants; v=0 interacts with $\Omega=2(v=0)$, v=1 with B $^3\Pi_0+(v=2)$. Ω -type doubling $\Delta v_{ef}(v=0) \approx +0.055 \times J(J+1)$.

^l $\Delta G(5/2) \approx 1100$.

^m Ω -type doubling $\Delta v_{ef} \left\{ \begin{array}{l} (v=0) \approx +0.022 \\ (v=1) \approx +0.060 \\ (v=2) \approx +0.095(\text{depert.}) \end{array} \right\} \times J(J+1) + \dots$

ⁿDeperturbed constants; $B_2 = 5.47$, $B_3 < 4.7$. D_0 refers to e levels, $D_1 \approx 3.2 \times 10^{-4}$, $D_2 \approx 6.8 \times 10^{-4}$. Perturbations by levels of b Δ_2 .

^oFrom a perturbation in B $^3\Pi_0+(v=0)$. Very uncertain.

^pDeperturbed constants; $B_2 = 5.83$; $D_1 = 4.95 \times 10^{-4}$, $D_2 \approx 7.8 \times 10^{-4}$. Perturbations by levels of A $^1\Sigma^+$, a ($^3\Sigma^+$), c 1.

^qv=2, 3, 4 perturbed by B $^3\Pi_0+(v=0, 1, 2)$. (Deperturbed) constants for v=2, ..., 6 are

$B_v = 6.199, 5.885, 5.540, 5.144, 4.576$.

$D_v(10^{-4} \text{ cm}^{-1}) = 4.92, 5.22, 6.3, 7.39, 8.8$.

$\Delta G(v+\frac{1}{2}) = 1427.0, 1319.7, 1166.8, 1020.5$.

^rPredissociation above v=0, J=0 (5) caused by an unstable $^3\Sigma^+$ state from Cu, $^2S + H, ^2S$. See also (6).

^s $\beta_e = +0.22 \times 10^{-4}$.

^tFrom a combination of Ringström's data for v=0, 1, 2 and Heimer's data for v=3, 4. $\omega_e v_e = +0.067$, $\gamma_e = +0.0015$, $\beta_e = -0.073 \times 10^{-4}$.

(1) Heimer, Heimer, ZP 84, 222 (1933)

(2) Grundström, ZP 98, 128 (1935).

(3) Heimer, ZP 95, 321 (1935).

(4) Heimer, Dissertation (Stockholm, 1937).

(5) Herzberg, Mundie, JCP 8, 263 (1940).

(6) Kleman, AF 6, 17 (1953).

(7) Bulewicz, Sugden, TFS 52, 1475 (1956).

(8) Loginov, OS(Engl. Transl.) 16, 220 (1964).

(9) Ringström, AF 32, 211 (1966).

(10) Ringström, CJP 46, 2291 (1968).

Cu²H: ^aFrom the value for Cu¹H.

^bA second level is observed at 2240.6 cm^{-1} above v=0, but could equally well be C1(v=3). It is perturbed, probably by b $\Delta_2(v=2)$. Approximate constants for the e levels are B = 2.85, D = 1.0×10^{-4} .

^c Ω -type doubling $\Delta v_{ef} = +0.0166 \times J(J+1) - \dots$

^d $H_0 = -19.6 \times 10^{-9}$ (average of e and f components).

^eConstants for e component. f component ($B_0 = 3.2558$, $D_0 = 1.270 \times 10^{-4}$, $v_{00} = 27152.83$) appears to be perturbed by a lower lying 0^- level of smaller B value. v=1 and 2 are perturbed by levels of a $^3\Sigma^+$ and b Δ_2 .

^fThe only observed transition is to v=1 (deperturbed) constants B = 3.102, D = 1.36×10^{-4} , v(1-0) = 27435.7. Evidence for additional levels comes from the observation of perturbations in B $^3\Pi_0+$ and C 1.

^gDeperturbed constants; $D_1 = 1.07 \times 10^{-4}$, $D_2 = 1.1 \times 10^{-4}$. Perturbations by levels of a $^3\Sigma^+$.

^h $\omega_e v_e = -0.570$.

ⁱ $B_4 = 3.0785$, $B_5 = 2.9633$, $B_6(\text{depert.}) = 2.83$.

^j $D_1, \dots, D_5(10^{-4} \text{ cm}^{-1}) = 1.16, 1.18, 1.28, 1.35, 1.44$.

^k $H_0 = +2.8 \times 10^{-9}$; $D_1 = 1.354 \times 10^{-4}$, $H_1 = 3.3 \times 10^{-9}$; $D_2 = 1.31 \times 10^{-4}$; $D_3 = 1.29 \times 10^{-4}$.

(1) Jeppesen, PR 50, 445 (1936).

(2) See ref. (4) of Cu¹H.

(3) See ref. (9) of Cu¹H.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$(^{63})\text{Cu}^1\text{H}^+ ?$		Fragments of a band system in the region $34500 - 45500 \text{ cm}^{-1}$. Lower state constants were reported in (1), but information is incomplete.							JAN 1975 (1)	
$^{63}\text{Cu}^{127}\text{I}$		$\mu = 42.068564_3$ $D_0^0 < 3.27 \text{ eV}^a$							AUG 1975 A	
E	$1\Sigma^+ (0^+)$ 24001.4	229.4 ₀ Z	0.95	0.0658 ^b	0.0003 ₆	(2.2)	2.46 ₈	E \leftrightarrow X, R	23983.8 ₀ Z	(1)(2)(5) (6)* (8)*
D	1Π (1) 22957.5	212.8 H	0.92	b				D \leftrightarrow X, R	22931.6 H	(1)(2)(8)*
C	$1\Sigma^+ (0^+)$ 21867.3	229.7 H	0.53	[0.0681] ^b			[2.42 ₆]	C \leftrightarrow X, R	21849.9 ₄ Z	(1)(2)(6) (8)*
c										
A	1Π (1) 19734.2	213.3 H	2.22	0.0676 ₁ ^d	0.0004 ₂	(2.7)	2.435	A \leftrightarrow X, R	19708.2 H	(1)(2)(10)*
X	$1\Sigma^+$ 0	264.5 Z	0.60	0.07328742	0.00028390 ₃ ^e	2.2439 ^f	2.338324	Microwave sp. ^g		(11)
$(^{63})\text{Cu}^{(7)}\text{Li}$		$(\mu = 6.3122532)$		$D_0^0 = 1.98 \text{ eV}^a$						APR 1975
$(^{63})\text{Cu}^{23}\text{Na}$		$(\mu = 16.838309_9)$		$D_0^0 = 1.7_9 \text{ eV}^a$						JAN 1975
$(^{63})\text{Cu}^{(58)}\text{Ni}$		$(\mu = 30.164639_6)$		$D_0^0 = 2.1_0 \text{ eV}^a$						JAN 1975

CuH⁺: (1) Mahanti, Nature 127, 557 (1931).

CuI: ^aThermochemical value (3).

^bRotational analyses of C-X and E-X by (6); analyses of C-X, D-X, E-X by (8) and of D-X by (7) are erroneous or doubtful. See also (9).

^cBands previously assigned to a B-X system are now known to be due to Cu₂ (4).

^dRecalculated from (10).

^e+ $3.12 \times 10^{-7}(v+\frac{1}{2})^2 - 1.3 \times 10^{-9}(v+\frac{1}{2})^3$.

^fH_e = - 2.288×10^{-15} .

^gAlso value for eqQ(¹²⁷I).

(1) Mulliken, PR 26, 1 (1925).

(2) See ref. (1) of CuBr.

(3) Brewer, Lofgren, JACS 72, 3038 (1950).

(4) See ref. (1) of Cu₂.

(5) Nair, Upadhy, Nature 211, 1170 (1966).

(6) Nair, Upadhy, CJP 44, 1267 (1966).

(7) Nair, Upadhy, CS 35, 593 (1966).

(8) Rao, Apparao, CJP 44, 2241, 2247 (1966).

(9) Nair, Rai, CJP 45, 2810 (1967).

(10) Pandey, Upadhy, Mohanty, IJP 42, 154 (1968).

(11) Manson, De Lucia, Gordy, JCP 62, 4796 (1975).

(12) Wu, Dows, JMS 58, 384 (1975)

CuLi: ^aThermochemical value (mass-spectrom.)(1).

(1) Neubert, Zmbov, JCS FT I 70, 2219 (1974).

CuNa: ^aThermochemical value (mass-spectrom.)(1).

(1) Piacente, Gingerich, ZN 28 a, 316 (1973).

CuNi: ^aThermochemical value (mass-spectrom.)(1).

(1) Kant, Strauss, Lin, JCP 52, 2384 (1970).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{63}\text{Cu}^{16}\text{O}$										AUG 1975 A
$\mu = 12.7533703_7$ $D_0^0 = 2.7_9 \text{ eV}^a$										(5)(9)
Unidentified transitions in matrix absorption ($F \leftarrow X?$) and fluorescence.										(12)
P $2\Pi_{3/2}$		[574] ^b		[0.384] ^b	0.005		[1.85 ₅] ^b	$P \rightarrow X_1$, R	25194 ^b	(12)
M $2\Pi_{3/2}$				[0.419] ^c			[1.77 ₆] ^c	$M \leftrightarrow X_1$, R	23898 ^c Z	(3)(8)(10)
I $2\Pi_{3/2}$		[608] ^d		[0.416] ^d	0.004 ₆		[1.78 ₃] ^d	$I \rightarrow X_1$, R	22449 ^d	(12)
H $2\Pi_{3/2}$		[557] ^d		[0.4176] ^d	0.005 ₆		[1.779 ₁] ^d	$H \rightarrow X_1$, R	22326 ^d	(12)
G $2\Sigma^{(-)}(\frac{1}{2})$	21618.6	[582.74]	Z (4.0)	0.41481 ^e	0.00370	7.24	1.7850 ₉	$G \rightarrow X_2^{f, f}$, R	21316.94 ^g Z 21593.98 ^g Z	(11)*
F $2\Pi_i$	21237 ^h	[600.8]	Z (4.4)	0.4121 ⁱ	0.0038	8	1.791 ₀	$F \rightarrow X$, R	21082.8 ^j Z	(4)* (8) (10)* (11)
E $2\Delta_{5/2}$	21058.0	733	H ^Q 5.5	0.4445 ^k	0.0036		1.724 ₄	$E \rightarrow X_1$, R	21104.1 H ^Q	(12)
Bands in the green region, partially analysed (13) in terms of a $2\Pi_i \rightarrow X$ $2\Pi_i$ transition.										(4)* (13)*
A $2\Sigma^{(+)}$	16491.3	[631.02]	Z (6.0)	0.43387 ^l	0.00475	7.93	1.7454 ₃	$A \leftrightarrow X_2^{f, f}$, R	16215.33 ^g Z 16492.37 ^g Z	(4)* (7)* (8)(10)*
X ₂ $2\Pi_{1/2}$	279.02 ^m	636.18	Z 4.36	0.44415 ⁿ	0.00449	8.4	1.7251 ₃	o		
X ₁ $2\Pi_{3/2}$	0	640.17	Z 4.43	0.44454	0.00456	8.5	1.7243 ₇			

CuO: ^aThermochemical value (mass-spectrom.)(1)(6).
^bLowest observed level and ΔG , vibrational numbering unknown. The observed transitions are $v=3$ at 23327 cm^{-1} , $v=4$ and $(v+1)-4$.
^cOne level only. Vibrational numbering uncertain; the authors in (4) suggest $v=1$. Perturbations.
^dThese are values of $\Delta G(\frac{3}{2})$, B_1 , r_1 , $v(1-0)$. $v=0$ not observed.
^eSpin doubling $\Delta v_{12} \begin{cases} (v=0) = + 0.1674 \\ (v=1) = + 0.1743 \end{cases} \times N(N+1) + \dots$
^f $G \rightarrow X_1$ is considerably weaker than $G \rightarrow X_2$. Relative branch intensities in both sub-bands are unusual.
^g $N'=0$ relative to $\{J''=0\}$.
^h $A_0 = - 6.24$, $A_1 = - 31.87$. Also J-dependent terms (10).
ⁱ $v=0$ perturbed. Λ -type doubling in $v=1$:
 $^2\Pi_{1/2}$, $\Delta v_{fe} = (-)[0.319_0(J+\frac{1}{2}) - \dots]$;
 $^2\Pi_{3/2}$, $\Delta v_{fe} = (-)[2.74 \times 10^{-5}(J-\frac{1}{2})(J+\frac{1}{2})(J+3/2) - \dots]$.
^j $J'=\frac{1}{2}$ relative to $J''=\frac{1}{2}$ (average of $\{F_1\}$ and F_2).
^k $v=0$ strongly perturbed.
^lSpin-doubling constants $\gamma_0 = - 0.1952$, $\gamma_1 = - 0.1908$.
^m $A_0 = - 276.11$, $A_1 = - 272.28$, $A_2 = - 268.69$; also J-dependent terms (10).
ⁿ Λ -type doubling in $^2\Pi_{1/2}$, $\Delta v_{fe} = (-)[0.014_8(J+\frac{1}{2}) - \dots]$ (average of $v=0, 1, 2$).
^oThe absence of an ESR spectrum attributable to matrix isolated CuO is compatible with a $^2\Pi$ ground state (9).

CuO (continued):

- (1) R. P. Burns, quoted in (2).
- (2) Cheetham, Barrow, AdHTC 1, 7 (1967).
- (3) Lagerqvist, Uhler, ZN 22 b, 551 (1967).
- (4) Antić-Jovanović, Pěšić, Gaydon, PRS A 307, 399 (1968).
- (5) Shirk, Bass, JCP 52, 1894 (1970).
- (6) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).
- (7) Antić-Jovanović, Pěšić, JP B 6, 2473 (1973).
- (8) Appelblad, Lagerqvist, JMS 48, 607 (1973).
- (9) Thompson, Easley, Knight, JPC 27, 49 (1973).
- (10) Appelblad, Lagerqvist, PS 10, 307 (1974).
- (11) Appelblad, Lagerqvist, CJP 53, 2221 (1975).
- (12) O. Appelblad, A. Lagerqvist, USIP Annual Report 1974 (May-75), and private communication.
- (13) Lefebvre, Pinchemel, Bacis, CJP 54, 735 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(^{63}\text{Cu}^{(32)}\text{S})$										
		$(\mu = 21.2007816)$		$D_0^0 = 2.8_0 \text{ eV}^a$						SEP 1976 A
A $2\Sigma^+(+)$	17946.1	375.2 ^b	H ^Q 3.6 ₆	[0.1806] ^c		[18]	[2.099]	A→X, R	$\frac{17493.1}{17925.7}$ $\frac{H^Q}{H^Q}$	(1)(4)
X $2\Pi_{(i)}$	433.4 0	413.4 415.0	$\frac{H^Q}{H^Q}$ 1.6 ₅ 1.7 ₅	[0.1891]		[18]	[2.051]			
$^{63}\text{Cu}^{121}\text{Sb}$										
		$\mu = 41.387622_9$								JAN 1975
				Additional sequences of R shaded bands in thermal emission at 13014, 13843, 14476, 15423, 15825, 16482 cm^{-1} .						(1)*
A	18511.7	222.7 ₁	H 0.86					A→X, R	18505.6 H	(1)
X ^a	0	234.8 ₃	H 0.73							
$^{63}\text{Cu}^{80}\text{Se}$										
		$\mu = 35.206516_8$		$D_0^0 = 2.5_5 \text{ eV}^a$						SEP 1976
A $2\Sigma^+(+)$	17960.4	253.0	H 2.74	[0.10169] ^b		[7.0]	[2.169 ₉]	A→X, R	$\frac{16344.37}{17935.32}$ $\frac{Z}{Z}$	(1)* (3)*
X $2\Pi_i$	1590.9 0	302.3 ₇	H 0.99	$\frac{[0.10775]^c}{[0.10774]}$		[5.9]	[2.1081]			
$(^{63}\text{Cu}^{(120)}\text{Sn})$										
		$(\mu = 41.269608_7)$		$D_0^0 = 1.8_0 \text{ eV}^a$						JAN 1975
$^{63}\text{Cu}^{130}\text{Te}$										
		$\mu = 42.393295_1$		$D_0^0 = 2.3_5 \text{ eV}^a$						OCT 1975
				Fragments of an additional system in the region 17200 - 18200 cm^{-1} .				(B→X)		(3)
A ^b	15991.92	200.58	H 2.009	0.0673 ₀	0.0005 ₂	3.41 ^c	2.431	A→(X), R	15965.55 H	(1)* (3)*
(X) ^b	0	252.67	H 0.701	0.0720 ₅	0.0002 ₈	2.65 ^d	2.349			

CuS: ^aThermochemical value (mass-spectrom.)(2)(3)(5).

^bAverage of Biron's (1) constants for the upper states of his systems A and B.

^cSpin-splitting constant $\gamma_0 = -0.0360$.

(1) Biron, CR 258, 4228 (1964).

(2) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).

(3) Uy, Drowart, TFS 67, 1293 (1971).

(4) Biron, CR B 274, 978 (1972); 281, 401 (1975).

(5) See ref. (6) of CuO.

CuSb: ^aNot certain that this is the ground state.

(1) Lefebvre, Houdart, CR B 273, 662 (1971).

CuSe: ^aThermochemical value (mass-spectrom.)(2).

^bSpin-splitting constant $\gamma_0 = -0.0022$.

^c Λ -type doubling, $\Delta v_{fe}(v=0) = (-)[0.0284(J+\frac{1}{2}) - \dots]$.

(1) Joshi, JMS 8, 79 (1962).

(2) See ref. (6) of CuO.

(3) Lefebvre, Bocquet, CJP 54, 1664 (1976).

CuSn: ^aThermochemical value (mass-spectrom.)(1).

(1) Ackerman, Drowart, Stafford, Verhaegen, JCP 36, 1557 (1962).

CuTe: ^aThermochemical value (mass-spectrom.)(2).

^b $\Omega' = \Omega''$.

^c $\beta_e = +0.14 \times 10^{-8}$.

^d $\beta_e = +0.01 \times 10^{-8}$.

(1) Maheshwari, Sharma, PPS 81, 898 (1963).

(2) See ref. (6) of CuO.

(3) Lefebvre, Bocquet, JP B 8, 1322 (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(164)Dy ¹⁹ F		($\mu = 17.0252779$)		$D_0^0 = 5.4_6 \text{ eV}^a$						JAN 1975
(164)Dy ¹⁶ O		($\mu = 14.5729973_4$)		$D_0^0 = 6.2_5 \text{ eV}^a$						JAN 1975 A (1)(2)* (3)
		Large number of mostly R shaded emission bands, 15900 - 19600 and 20800 - 23500 cm^{-1} . Tentative vibrational analysis by (1); uncertain.								
(166)Er ¹⁹ F		($\mu = 17.0466290$)		$D_0^0 = 5.8_3 \text{ eV}^a$						JAN 1975
(166)Er ¹⁶ O		($\mu = 14.5886378_7$)		$D_0^0 = 6.3_0 \text{ eV}^a$						JAN 1975 A (1)* (2)
		V and R shaded emission bands in the regions 17200 - 18500 and 19200 - 20400 cm^{-1} .								
(153)Eu ¹⁹ F		($\mu = 16.8989393$)		$D_0^0 = 5.4_2 \text{ eV}^a$						OCT 1975 (2)
		Emission in the region 14000 - 33000 cm^{-1} , maximum at 26000 cm^{-1} .								
(153)Eu ¹⁶ O		($\mu = 14.4803335_6$)		$D_0^0 = 4.8_0 \text{ eV}^a$						OCT 1975 A (1)* (5)(6) (4)
		Emission spectrum from 14000 to 25000 cm^{-1} .								
X	0	[668.0] ^b							IR abs. sp. ^b	
(153)Eu ⁽³²⁾ S		($\mu = 26.4434070$)		$D_0^0 = 3.7_1 \text{ eV}^a$						JAN 1975
(153)Eu ⁽⁸⁰⁾ Se		($\mu = 52.486909_4$)		$D_0^0 = 3.0_8 \text{ eV}^a$						JAN 1975
(153)Eu ⁽¹³⁰⁾ Te		($\mu = 70.238662$)		$D_0^0 = 2.4_5 \text{ eV}^a$						JAN 1975

DyF: ^aThermochemical value (mass-spectrom.)(1).

(1) Zmbov, Margrave, JPC 70, 3379 (1966).

DyO: ^aThermochemical value (mass-spectrom.)(4), recalc.(5).

(1) Piccardi, SA 1, 533 (1941).

(2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(3) Mavrodineanu, Boiteux, "Flame Spectroscopy", Wiley (1965).

(4) Ames, Walsh, White, JPC 71, 2707 (1967).

(5) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

ErF: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (1) of DyF.

ErO: ^aThermochemical value (mass-spectrom.)(3), recalc.(4).

(1) See ref. (2) of DyO.

(2) Herrmann, Alkemade, "Chemical Analysis by Flame Photometry", Wiley-Interscience (1963).

(3) See ref. (4) of DyO.

(4) See ref. (5) of DyO.

EuF: ^aThermochemical value (mass-spectrom.)(1). From the short-wavelength cutoff of the chemiluminescence spectrum (2) obtain $D_0^0 \geq 5.62$ eV.

(1) Zmbov, Margrave, JINC 29, 59 (1967).

(2) Dickson, Zare, CP 7, 361 (1975).

EuO: ^aThermochemical value (mass-spectrom.)(7). Considerably higher values (5.7₂ eV) in (2)(3)(6).

^bIn Ar matrix at 15 K. For Eu¹⁸⁰ at 633.7 cm⁻¹. Derived constants are $w_e = 671.8$, $w_e x_e = 1.9$ (4).

(1) See ref. (2) of DyO.

(2) See ref. (4) of DyO.

(3) See ref. (5) of DyO.

(4) Gabelnick, Reedy, Chasanov, JCP 60, 1167 (1974).

(5) Edelstein, Eckstrom, Perry, Benson, JCP 61, 4932 (1974).

(6) See ref. (2) of EuF.

(7) Hildenbrand, Murad, ZN 30 a, 1087 (1975).

EuS: ^aThermochemical value (mass-spectrom.)(1), recalc.(2).

(1) See ref. (5) of DyO.

(2) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

EuSe: ^aThermochemical value (mass-spectrom.)(2). Based on $D_0^0(\text{Se}_2) = 3.411$ eV; (1) prefer $D_0^0(\text{Se}_2) = 3.164$ eV.

(1) Barrow, Chandler, Meyer, PTRSL A 260, 395 (1966).

(2) See ref. (2) of EuS.

EuTe: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (2) of EuS.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{19}\text{F}_2$		$\mu = 9.4992023$ $D_0^0 = 1.602 \text{ eV}^a$ I.P. = 15.686 eV^b							JUL 1976 A	
		Many strong absorption bands observed and partially analyzed up to 126000 cm^{-1} , heavily perturbed and not assigned. ^c							(19)*	
K $^1\Pi_u$				[1.040] ^d			[1.306]	K ← X, V 116855.72 Z	(16)(19)*	
J $^1\Pi_u$ (4pσ)	116409	[1032.6] Z		[1.041]	e		[1.306]	J ← X, V 116469.4 Z	(19)*	
I $^1\Sigma_u^+$ (4pπ)	113841	[1108.92] Z	f	[0.8009]	g	[1.8] ^h	[1.488] ₆	I → f, R 17081.6 ⁱ H	(7)* (8)(19)	
								I → F, R 20732 ^j H	(7)* (8)(19)	
								I ↔ X, ^k R 113940.24 Z	(14)(16)(19)*	
H $^1\Pi_u$ (3pσ)	105520.14	1088.19 Z	9.875	1.021 ^l	0.014		1.318	H ← X, V 105606.27 Z	(16)(19)	
h $^3\Pi_{1u}$ (3pσ)(104904)		(1100) ^m		1.022 ⁿ	0.016		1.318	h ← X, V 104998.7 Z	(19)	
G $^1\Sigma_u^+$ (3pπ)(104300)		Inferred from strong perturbations of the higher vibrational levels of C $^1\Sigma_u^+$.							(19)	
E ($^1\Sigma_u^+$)	≤100912	[196.3] ^o Z	(0.96)	[0.194] ^o			[3.02] ^o	E ← X, R 100555.5 ^o Z	(19)*	
D ($^1\Sigma_u^+$)	≤98756	[221.6] ^o Z	(1.22)	[0.207] ^o			[2.93] ^o	D ← X, R 98411.9 ^o Z	(19)*	
f ($^3\Pi_{1g}$) (3sσ)	[97314] ^p	p		[1.005] ^p			[1.329] ^p			
C $^1\Sigma_u^+$	≤93499	[493.2] ^q Z		[0.484] ^q			[1.915] ^q	C ↔ X, R 93290.4 ^q Z	(19)*	
F $^1\Pi_g$ (3sσ)	93099	1133.34 ^r H	9.17 ₃	1.047 ^r	0.012		1.302			
A $^1\Pi_u$		Continuous absorption with maximum at 35000 cm^{-1} .						A ← X,	(4)(5)	
a $^3\Pi_{0+u}$		Continuous absorption with maximum at 25500 cm^{-1} .						a ← X, ^s	(4)(5)	
X $^1\Sigma_g^+$	0	916.64 Z	11.236 ^t	0.89019	0.013847 ^u	3.3	1.41193	Raman sp.	(2)(9)(18) (20)	
								Mol. beam magn. reson. ^v	(6)	
								Ab initio calc.	(13)	

- F_2 : ^aFrom the observed vibrational levels of the ground state (19); the highest observed level (presumably the last stable level) is at 12830.38 cm^{-1} . Shock tube experiments of (15) give the same value within $\pm 0.05 \text{ eV}$; see also the earlier work of (3)(5a)(10).
- ^bFrom photoionization (12). Photoelectron spectra (11) give 15.70 eV .
- ^cThe assignments to two Rydberg series by (16) are questioned by (19).
- ^d B_Q ; $B_{PR} = 1.034$.
- ^e $B_2 = 0.9916$.
- ^f $\Delta G(3/2) = 754.06$, $\Delta G(5/2) = 553.78$, $\Delta G(7/2) = 733.01$; strongly perturbed, not certain whether one or two electronic states are involved.
- ^g $B_1 = 0.8129$, $B_2 = 0.8980$, $B_3 = 0.8946$, $B_4 = 0.891$; see ^f.
- ^h $D_v(v=1\dots 4, 10^{-6} \text{ cm}^{-1}) = 4.0, 14.0, -2.6, -50.0$.
- ⁱThe lower state vibrational numbering of this band is unknown, see ^p.
- ^j v uncertain, see ^r.
- ^kFour of the strongest absorption bands; in emission only bands with $v=0$ and 1 and very weakly $v=2$.
- ^lFrom Q branches, $B_Q - B_{PR} \approx +0.004$. $v'=0, 1, 2, 3$ analyzed, a weak and highly perturbed band at 911 Å (109770 cm^{-1}) may be $4-0$.
- ^mEstimated from the $0-0$ and $2-0$ ($v_0 = 107069.4$) bands.
- ⁿFrom Q branches; $B_Q - B_{PR} = +0.005$. $v=0$ strongly perturbed.
- ^o(Deperturbed) constants determined from the lowest observed levels; vibrational numbering unknown. Only those levels which interact strongly with $C^1\Sigma_u^+$ have been found in absorption. It is possible that D and E are not two independent states.

- ^pFrom $I \rightarrow f$ (7); vibrational numbering unknown. The assignments of (8) suggest the existence of additional levels at 1058 below and 1044 cm^{-1} above the single level reported by (7).
- ^qConstants for the lowest observed level, vibrational numbering unknown ($v=n$). In absorption levels up to $v = n+30$ have been observed. Numerous perturbations by levels of D and E (interaction matrix elements $\approx 10 \text{ cm}^{-1}$); a much stronger interaction with G affects levels having $v \geq n+25$. For details see Table 5 of (19).
- ^rVibrational numbering uncertain. Extensive perturbations. Strong predissociation leading to line broadening in $I \rightarrow F$ bands having $v'' = 1, 2, 4, 5, 6, 8$; bands with $v'' = 3, 7$ are sharp.
- ^sThe existence of the $a \leftarrow X$ absorption becomes clear only after subtraction of the much stronger effect of the $A \leftarrow X$ absorption from the observed absorption intensities (5). It is generally assumed that the $^3\Pi_0 + u$ state has a minimum but no discrete absorption or emission has been observed, see (1). (17) predict a dissociation energy $D_e = 3300 \text{ cm}^{-1}$ and $r_e = 1.9 \text{ Å}$ for this state.
- ^t $w_{ey_e} = -0.113$. These constants represent only the lowest nine levels (i.e. $v \leq 8$) (19). Levels have been observed up to $v=22$; this last level lies only 90 cm^{-1} below the extrapolated limit.
- ^u $+0.0001179(v+\frac{1}{2})^2 - 0.000020_3(v+\frac{1}{2})^3$, representing $B_0 \dots B_{12}$.
- ^vRotational gyromagnetic ratio $g_J = -0.120_8 \mu_N$, (nuclear) spin-rotation and spin-spin interaction constants $c = -157.3 \text{ kHz}$, $d = 8.0 \text{ kHz}$.

References on page 217 .

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{19}\text{F}_2^+$		$D_0^0 = 3.33_9 \text{ eV}^a$							JUL 1976 A	
		<u>Ab initio</u> calculations (3) predict several further stable states. Ground state calc. (7).								
B ($^2\Sigma_g^+$) (43000)		From the photoelectron spectrum; uncertain observation.							(4)	
A	$^2\Pi_{u,i}$ (22755) 22484.8 ^b	520.4 ^b	7.3 ^b					A \rightarrow X, ^c R 22139 22208.8 ^b H	(2)	
X	$^2\Pi_{g,i}$ 340 ^d 0	1073.3 ^b H	9.13 ^b	1.015 ^e	0.010		1.322			
$^{19}\text{F}_2^-$		$D_0^0 = 1.28 \text{ eV}^a$ I.P. = 3.08 eV ^b							JUL 1976	
F	(120490)	1210 ^c	60						(4)	
E	($^2\Pi_g$) (115300)	1050 ^c							(4)	
X	$^2\Sigma_u^+$ 0	(510) ^d		(0.50) ^d			(1.8 _g) ^d			

F_2^+ : ^aFrom $D_0^0(\text{F}_2)$, I.P. (F_2), and I.P. (F).

^bFrom the R heads in the 3/2-3/2 sub-system. The (arbitrary) lower state vibrational numbering of (2) has been reduced by 5 leading to better agreement with the excitation energy of 2.70 eV (21800 cm^{-1}) and the ground state vibrational frequency found by photoelectron spectroscopy (4)(5); see also (6).

^cBands attributed to this system by (1) are probably all due to F_2 (I \rightarrow F), see (2).

^dFrom the photoelectron spectrum (4). At slightly lower resolution (5) find 240 cm^{-1} .

^eRevised vibrational numbering, see ^b.

F_2^+ (continued):

- (1) Stricker, ZN 21 a, 1518 (1966).
- (2) See ref. (7) of F_2 .
- (3) Balint-Kurti, MP 22, 681 (1971).
- (4) See ref. (11) of F_2 .
- (5) Potts, Price, TFS 67, 1242 (1971).
- (6) See ref. (16) of F_2 .
- (7) Ellis, Banyard, Tait, Dixon, JP B 6, L233 (1973).

- F_2^- : ^aFrom $D_0^0(F_2)$ and the electron affinities of F_2 (3.08 eV) and F (3.399 eV).
^bFrom endoergic charge transfer reactions (1).
^cTwo progressions of resonances in the electron transmission current starting at 11.25 and 11.90 eV. They indicate the existence of doubly excited (preionizing) states of F_2^- having the $F\ 1\Pi_g$ and $f\ 3\Pi_g$ Rydberg states of F_2 as parent states and $X\ 2\Pi_g$ of F_2^+ as grandparent.
^dTheoretical values from MO-SCF calculations (2), $D_e = 1.66$ eV. Multiconfiguration valence bond calculations (3) give $\omega_e = 293$, $\omega_e x_e = 1$, $B_e = 0.425$, $r_e = 2.04\ \text{\AA}$, $D_e = 1.06$ eV. See also (3a)(matrix Raman sp.).

F_2^- (continued):

- (1) Chupka, Berkowitz, Gutman, JCP 55, 2724 (1971).
- (2) Gilbert, Wahl, JCP 55, 5247 (1971).
- (3) Copsey, Murrell, Stamper, MP 21, 193 (1971).
- (3a) Howard, Andrews, JACS 95, 3045 (1973).
- (4) Spence, PR A 10, 1045 (1974).

F_2 (continued):

- (1) Nathans, JCP 18, 1122 (1950).
- (2) Andrychuk, CJP 29, 151 (1951).
- (3) Barrow, Caunt, PRS A 219, 120 (1953).
- (4) Steunenbergh, Vogel, JACS 78, 901 (1956).
- (5) Rees, JCP 26, 1567; 27, 1424 (erratum) (1957).
- (5a) Stamper, Barrow, TFS 54, 1592 (1958).
- (6) Ozier, Crapo, Cederberg, Ramsey, PRL 13, 482 (1964).
- (7) Porter, JCP 48, 2071 (1968).
- (8) Stricker, Krauss, ZN 23 a, 486 (1968).
- (9) Claassen, Selig, Shamir, AS 23, 8 (1969).
- (10) DeCorpo, Steiger, Franklin, Margrave, JCP 53, 936 (1970).

F_2 (continued):

- (11) Cornford, Frost, McDowell, Ragle, Stenhouse, JCP 54, 2651 (1971).
- (12) Berkowitz, Chupka, Guyon, Holloway, Spohr, JCP 54, 5165 (1971).
- (13) Das, Wahl, JCP 56, 3532 (1972).
- (14) Di Lonardo, Douglas, JCP 56, 5185 (1972).
- (15) Blauer, Solomon, JCP 57, 3587 (1972).
- (16) Gole, Margrave, JMS 43, 65 (1972).
- (17) Child, Bernstein, JCP 59, 5916 (1973).
- (18) Stricker, Hochenbleicher, ZN 28 a, 27 (1973).
- (19) Colbourn, Dagenais, Douglas, Raymonda, CJP 54, 1343 (1976).
- (20) Edwards, Good, Long, JCS FT II 72, 984 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{56}\text{Fe}_2)$ C B A X	0	$(\mu = 27.967467_0)$ Continuous absorption with maximum at 24120 cm $^{-1}$. (218) ^c (194) ^c						$C \leftarrow X,^b$ $B \leftarrow X,^b$ $A \leftarrow X,^b$	(21095) ^d (18355) ^d	MAR 1976 (2) (2) (2)
$(^{56}\text{Fe}^{(79)}\text{Br})$		$(\mu = 32.734036_2)$ Very diffuse absorption feature at 40890 cm $^{-1}$. Narrow group of absorption bands ^a in the region 28100 - 28400 cm $^{-1}$. Bands in the region 26600 - 27400 cm $^{-1}$; $w' \approx 315$, $w'' \approx 304$, possibly $^4\Pi \leftrightarrow ^4\Sigma$. V and R shaded emission bands in the region 15400 - 17500 cm $^{-1}$, tentative assignments to four systems.						$^4\Pi \leftrightarrow ^4\Sigma$ V	27064.9 H 27007.8 H 26935.1 H 26832.1 H	MAR 1976 (5) (5) (1)(2)(4)(5) (2)(3)
$(^{56}\text{Fe}^{35}\text{Cl})$ C ($^4\Pi$) B ($^6\Pi$) $x_2 +$ A ($^4\Pi$) $x_1 +$	 <									

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(56) Fe^{35}Cl (continued)										
A' ($^4\Pi$)		Complex system in the region $20000 - 21000 \text{ cm}^{-1}$; $w' = 370$, $w'' = 395$.						$(A' \rightarrow X_1)$, R	20549.3 H 20484.5 H 20429.0 H 20378.0 H	(5)
		Fragments of an emission system; $w' \approx 405$, $w'' \approx 394$.						V	17379	(5)
		Tentative assignments of emission bands in the regions $16480 - 16720$ and $15250 - 15750 \text{ cm}^{-1}$.						V	(16486)	(3)(5)
								V_R	(15443)	(3)(5)(8)
X_2 ($^6\Sigma$)	x_2^b	407.2 H	1.4							
X_1 ($^4\Sigma$)	x_1^b	(409.9) ^a H	(2.2)							

Fe_2 : ^aThermochemical value (mass-spectrom.)(1).
^bIn Ar matrices at 10 K.
^cLong upper state progression.
^dLowest observed level, vibrational numbering unknown.
(1) Lin, Kant, JPC 73, 2450 (1969).
(2) De Vore, Ewing, Franzen, Calder, CPL 35, 78 (1975).

FeBr : ^aResembling the B- X_2 system of FeCl .
(1) Miescher, HPA 11, 463 (1938).
(2) Mesnage, AP(Paris) 12, 5 (1939).
(3) Reddy, JSIR B 18, 188 (1959).
(4) Rao, Rao, JP B 3, 725 (1970).
(5) See ref. (3) of FeF .

FeCl : ^aVibrational constants from (9). An earlier analysis (4) of A- X_1 gave $w_e' = 431.0$, $w_e' x_e' = 2.9$, $w_e'' = 397.0$, $w_e'' x_e'' = 1.6$.
^bIt is not certain whether X_1 or X_2 is the ground state.
(1) Mesnage, CR 201, 389 (1935).
(2) See ref. (1) of FeBr .
(3) See ref. (2) of FeBr .
(4) Müller, HPA 16, 3 (1943).
(5) Reddy, Rao, JMS 4, 16 (1960).
(6) Rao, Rao, CS 38, 87 (1969).
(7) Rao, Rao, JP B 3, 878 (1970).
(8) Rao, Rao, Rao, CS 39, 392 (1970).
(9) Rao, Rao, IJPAP 9, 102 (1971).
(10) See ref. (3) of FeF .

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(⁵⁶Fe¹⁹F										
C	x + (42743)	($\mu = 14.1815983$) (694) H (7)						C \leftrightarrow (X), V 42751	H	FEB 1975 (3)* (1) (2)(3)* (2)(3)*
(X)	x	Single sequence of bands near 32060 cm^{-1} , in emission only. Narrow group of bands ^a , $30900 - 31200 \text{ cm}^{-1}$, in em. and abs.. Narrow group of bands ^b near 30240 cm^{-1} , in em. and abs.. (678) H (7)						(R) (V) (V)		
(⁵⁶Fe(⁷⁴Ge										
		($\mu = 31.841213_8$)		$D_0^0 = 2.1_4 \text{ eV}^a$						JAN 1975
(⁵⁶Fe¹H										
(⁵⁶Fe²H										
		($\mu = 0.98998780$) ($\mu = 1.94409920$)								AUG 1975 A (2)* (3) (4)
		Complex abs. and em. spectra, $18500 - 19200$ and $19900 - 21300 \text{ cm}^{-1}$. No analysis. Additional band at 10100 cm^{-1} . Theoretical calculations (1)(5) predict a $^6\Sigma^+$ or $^6\Delta$ ground state.								
(⁵⁶Fe¹⁶O										
		($\mu = 12.4381536_7$)		$D_0^0 = 4.2_0 \text{ eV}^a$		I.P. = 8.7_1 eV^b				JUN 1977
		Single band, in emission and absorption.								
c	26441	[545] H						c \rightarrow A ^c , R 41480	H	(8)* (9)(12)*
c'	23569	[535] H	Fragments of an emission system, $18500 - 20000 \text{ cm}^{-1}$.					c' \rightarrow A ^c , R 22326	H	(1)(3)(19)
								R 19449	H	(19)
b	21962 (21865)	[667] H [(661)] H		[0.4717] ^d		[1.695]		b ^e \leftrightarrow A ^c , R 17908	H	(1)(2)* (7)* (8)(9)(14)
								R 17808	H	(19)
a	21245	820 H 1		[0.497] ^f		[1.65] ₁		a ^g \leftrightarrow A ^c , R 17267	H	(1)(2)* (7)* (8)(9)(19)
B (⁵ Π)	14404	650 ^h H 5	Large number of emission bands, $7100 - 15000 \text{ cm}^{-1}$; tentative vibrational analyses.					B \rightarrow A ^c , R 10340	H	(5)(19)
A ⁵ Σ^+ i	3948	880.53 ^d Z	4.63	0.5127 ₁ ^d	0.0037 ₆	[0.6] ₆	1.6259	B \rightarrow X, R 14245	H	(3)(19)(21)
X ⁵ Δ i	0	965 ^h H					(1.57) ^k	$T_0 = 3905^j$		
(⁵⁶Fe¹⁶O⁻										
X	0	740 ⁿ		$D_0^0 = 4.2_3 \text{ eV}^m$		I.P. = 1.49_2 eV^n	(1.63) ^k			JUN 1977

FeF: ^aSimilar in appearance to the B-X₂ system of FeCl.
^bSimilar in appearance to the A-X₁ system of FeCl.
 Additional bands at 29580 cm⁻¹ (2) suggest $\Delta G''(\frac{1}{2}) \approx 660$.
 (1) Barrow, Carroll, unpublished, quoted in DONNSPEC.
 (2) Senior, Barrow, unpublished, quoted in DONNSPEC.
 (3) Brinton, Callear, JCS FT II 70, 203 (1974).

FeGe: ^aThermochemical value (mass-spectrom.)(1).
 (1) Kant, Strauss, JCP 49, 3579 (1968).

Fe¹H, Fe²H:

- (1) Walker, Walker, Kelly, JCP 57, 2094 (1972).
- (2) Carroll, McCormack, ApJ (Part 2) 177, L33 (1972).
- (3) Smith, PRS A 332, 113 (1973).
- (4) Klynning, Lindgren, USIP Report 73-20 (1973).
- (5) Scott, Richards, JCP 63, 1690 (1975).

FeO, FeO⁻:

- ^aThermochemical value (mass-spectrom.)(10)(15)(20). See also (4)(6).
- ^bElectron impact appearance potential (20).
- ^cThe similarity of the vibrational constants suggests a common lower state for the five systems. Uncertain.
- ^dFrom the rotational analysis (14) of four bands of the short-wavelength component of b-A. They appear to be the $\Omega' = \Omega'' = 0$ subbands of a quintet or septet $\Sigma - \Sigma$ transition. An earlier analysis by (11) is incorrect.
- ^eLifetime $\tau \approx 500$ ns (19).
- ^fRotational analysis using tunable-laser excited fluorescence spectroscopy (19).
- ^gLifetime $\tau \approx 450$ ns (19).
- ^hFrom a re-analysis of B→X by (21). The FeO⁻ photoelectron sp.(21) gives a ground state frequency of 970 ± 60 cm⁻¹.
- ⁱSymmetries assigned (21) on the basis of ab initio calculations (18).

FeO, FeO⁻ (continued):

- ^jFrom 0-0 band assignments for B→X (21) and B→A (5)(19). From the FeO⁻ photoelectron sp. (21) obtain 3990 ± 100 cm⁻¹.
- ^kEstimated (21) from relative vibrational intensities in the photoelectron spectrum of FeO⁻.
- ^lThe IR transition strength measured at 880 cm⁻¹ (16)(17) requires re-interpretation in view of the recent re-assignment of the low-lying states (21).
- ^mFrom D₀⁰(FeO) and the electron affinities of FeO and O.
- ⁿFrom the laser photoelectron spectrum of FeO⁻ (21).
- (1) Rosen, Nature 156, 570 (1945).
- (2) Delsemme, Rosen, BSRSL 14, 70 (1945).
- (3) Malet, Rosen, BSRSL 14, 377 (1945).
- (4) Brewer, Mastik, JCP 19, 834 (1951).
- (5) Bass, Benedict, ApJ 116, 652 (1952).
- (6) Lagerqvist, Huldt, ZN 8 a, 493 (1953).
- (7) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (8) Callear, Norrish, PRS A 259, 304 (1960).
- (9) Bass, Kuebler, Nelson, JCP 40, 3121 (1964).
- (10) Burns (1966), quoted in (13).
- (11) Dhumwad, Narasimham, PIAS A 64, 283 (1966).
- (12) Callear, Oldman, TFS 63, 2888 (1967).
- (13) Cheetham, Barrow, AdHTC 1, 7 (1967).
- (14) Barrow, Senior, Nature 223, 1359 (1969).
- (15) Balducci, De Maria, Guido, Piacente, JCP 55, 2596 (1971).
- (16) Von Rosenberg, Wray, JQSRT 12, 531 (1972).
- (17) Fissan, Sulzmann, JQSRT 12, 979 (1972).
- (18) Bagus, Preston, JCP 59, 2986 (1973).
- (19) West, Broida, JCP 62, 2566 (1975).
- (20) Hildenbrand, CPL 34, 352 (1975).
- (21) Engelking, Lineberger, JCP 66, 5054 (1977).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$(^{56}\text{Fe}^{(32)}\text{S})$		$(\mu = 20.3437228)$		$D_0^0 = 3.3_1 \text{ eV}^a$						JAN 1975
$(^{56}\text{Fe}^{(28)}\text{Si})$		$(\mu = 18.6491827)$		$D_0^0 = 3.0_4 \text{ eV}^a$						JAN 1975
$^{19}\text{F}^{16}\text{O}$ x $^2\Pi$ 0		$\mu = 8.6838822_5$ [1028.7] ^c	$D_0^0 = 2.2_3 \text{ eV}^a$ (5.15) ^d	$I.P. = 12.7_9 \text{ eV}^b$ (1.104) ^d	(0.0097) ^d		(1.32 ₆) ^d			JUL 1976
$(^{69,71}\text{Ga}_2)$		$(\mu = 34.955426_7)$		$D_0^0 = 1.4_0 \text{ eV}^a$						JUL 1976 (3)
		R shaded emission bands in the region 18200 - 21700 cm^{-1} ; $w \approx 165$.								

GaAs, GaBi See p. 226.

$^{69}\text{Ga}^{81}\text{Br}$		$\mu = 37.220586_4$ $D_0^0 = 4.3_1 \text{ eV}^a$					JUL 1976
C	1_{Π} (36000)	Diffuse absorption bands (fluctuation b.) indicating a shallow upper state potential curve.				$G \leftarrow X$, 37310 ^b	(1)
B	3_{Π_1} 28532.0	271.6 ^c	H	2.50		$B \leftrightarrow X$, V 28535.9	H (1)(5)*
A	3_{Π_0+} 28161.8	272.2 ^c	H	2.53		$A \leftrightarrow X$, V 28166.0	H (1)(5)*
X	1_{Σ^+} 0	263.0 ^c	H	0.81	0.081839 ₃ 0.0003207 (0.32) ^d 2.35248	Microwave sp.	(2)
$^{69}\text{Ga}^{35}\text{Cl}$		$\mu = 23.1990149$ $D_0^0 = 4.92 \text{ eV}^a$					JUL 1976
		Continuous absorption at 41200 and near 47600 cm^{-1} .					(1)(2)
C	1_{Π} (40261)	[120] ^b	H			$G \leftarrow X$, R 40139	H (1)(2)*
B	3_{Π_1} 29859.4	395.3	H	2.5	[0.1568 ₆] ^c	$B \leftrightarrow X$, V 29874.0 ₃ ^c	Z (1)(2)*
A	3_{Π_0+} 29527.2	395.3	H	2.3 ^d	[0.1577 ₉] ^e	$A \leftrightarrow X$, V 29541.9	(Z) (1)(2)*
X	1_{Σ^+} 0	365.3 ^f	H	1.2	0.1499045 0.0007936 ^g (1.01) ^h 2.201690	Microwave sp. ⁱ	(3)(7)

FeS: ^aThermochemical value (mass-spectrom.)(1)(2).

(1) Marquart, Berkowitz, JCP 39, 283 (1963).

(2) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).

FeSi: ^aThermochemical value (mass-spectrom.)(1).

(1) Vander Auwera-Mahieu, McIntyre, Drowart, CPL 4, 198 (1969).

FO: ^aIndirectly from the difference between the electron impact appearance potentials of FO^+ from FO and F_2O (4) and the known heat of atomization of F_2O ; see also (2)(5).
^bPhotoionization mass-spectrometry of F_2O (7). See also (2).
^cFrom matrix IR absorption and Raman spectra in Ar (1)(3) (6). (2) suggest a corrected gas phase frequency of 1050.
^dTheoretical calculations (2).

(1) Arkell, Reinhard, Larson, JACS 87, 1016 (1965).

(2) O'Hare, Wahl, JCP 53, 2469 (1970).

(3) Andrews, Raymond, JCP 55, 3078 (1971).

(4) Clyne, Watson, CPL 12, 344 (1971).

(5) Levy, JCP 56, 1415 (1972).

(6) Andrews, JCP 57, 51 (1972).

(7) Berkowitz, Dehmer, Chupka, JCP 59, 925 (1973).

Ga₂: ^aThermochemical value (mass-spectrom.)(1)(2)(4).

(1) Drowart, Honig, BSCB 66, 411; JPC 61, 980 (1957).

(2) Chupka, Berkowitz, Giese, Inghram, JPC 62, 611 (1958).

(3) Ginter, Ginter, Innes, JPC 69, 2480 (1965).

(4) Gingerich, Blue, 18th Annual Conference on Mass-Spectrometry and Allied Topics, San Francisco (June 1970), paper F2.

GaBr: ^aLimit from the analysis of the fluctuation bands, and extrapolation of vibrational levels in $^3\Pi_0+$ and $^3\Pi_1$; for correlation with atomic products see (3). Flame photometry (4) gives 4.4₅ eV.

^bVertical transition.

^cAnalysis of (1). (5) revised some of the vibrational assignments and gave constants for $^{69}\text{Ga}^{79}\text{Br}$.

^dCalculated from $4B_0/w_e^2$.

(1) Miescher, Wehrli, HPA 6, 458 (1933); 7, 331 (1934).

(2) Barrett, Mandel, PR 109, 1572 (1958).

(3) Barrow, TFS 56, 952 (1960).

(4) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(5) Savithry, Rao, Murty, Rao, Physica 75, 386 (1974).

GaCl: ^aFrom spectroscopic evidence concerning $\text{C}^1\Pi$, see (4). Good agreement with the flame photometric value of (6).
^bBands with $v'=1$ are diffuse on account of predissociation.
^cRecalculated by (5) from data in (2).
^d $w_e y_e = + 0.015$.

^e $B'_0 - B''_0$ redetermined from the differences between consecutive lines in the R and P branches measured by (2).

^f $\Delta G(\frac{1}{2}) = 363.32$ from band origins (5).

^g $\gamma_e = + 1.8_0 \times 10^{-6}$.

^hSee ^d of GaBr.

ⁱ $\text{eqQ}(^{69}\text{Ga}) = - [92.4_0 - 0.6_8(v+\frac{1}{2})]$ MHz,

$\text{eqQ}(^{35}\text{Cl}) = - [13.2_0 + 0.2_0(v+\frac{1}{2})]$ MHz (7).

(1) See ref. (1) of GaBr.

(2) Levin, Winans, PR 84, 431 (1951).

(3) See ref. (2) of GaBr.

(4) See ref. (3) of GaBr.

(5) Bartky, JMS 5, 206 (1960); 6, 275 (erratum) (1961).

(6) See ref. (4) of GaBr.

(7) Tiemann, Grasshoff, Hoeft, ZN 27 a, 753 (1972).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{69}\text{Ga}^{19}\text{F}$											
		$\mu = 14.8932747$	$D_0^0 = 5.98 \text{ eV}^a$						JUL 1976		
C	1Π	47365.7	542.3 ₅ (Z)	9.5 ₅ ^b	(0.358)	(0.0053 ₅) ^c	(1.778)	C \leftrightarrow X, R _V	47324.1 (Z)	(1)* (2)(3)	
B	$3\Pi_1$	33427.8	662.1 Z	1.45 ^d	0.3719 ₈ ^{ef}	0.0030 ₂	1.7444	B \leftrightarrow X, V	33448.1 ₂ Z	(1)* (2)(3)	
A	$3\Pi_0^+$	33105.5	663.0 ₂ Z	2.18 ^g	0.3709 ₈ ^e	(0.0030 ₂)	1.7467	A \leftrightarrow X, V	33126.1 ₇ Z	(1)* (2)(3)	
X	$1\Sigma^+$	0	622.2 Z	3.2	0.3595161	0.0028642 ^h	0.50	1.774369	Microwave sp. ⁱ	(6)(7)	
$^{69}\text{Ga}^1\text{H}$											
		$(\mu = 0.99330124)$	$D_0^0 < 2.84 \text{ eV}^a$						JUL 1976		
		Open-structure absorption bands in the region 41650 - 46300 cm^{-1} , provisionally ascribed to Ga^1H .							(1)		
A	1Π				[5.1] ^{bc}		[1.8 ₂]	A \leftrightarrow X, R	23714 H ^Q	(2)(3)(6)	
a	$3\Pi_2$				[6.811]		[620] ^d	[1.578 ₅]	\rightarrow X, V	17909.43 Z	(3)*
	$3\Pi_1$	17622.0 ₁	1631.1 ₇ Z	58.2 ₂ ^e	6.692 ^f	0.326 ^g	489 ^h	1.592 ₅	\leftrightarrow X, V _R	17626.84 Z	(2)(3)*
	$3\Pi_0^+$	17337.08	1640.54 Z	62.72 ⁱ	6.394 ^f	0.276 ^j	262 ^k	1.629 ₂	\leftrightarrow X R _V	17345.78 Z	(2)(3)*
	$3\Pi_0^-$	17333	[1492.5] Z	^l	6.358	0.220 ^m	[243] ⁿ	1.633 ₈	\rightarrow X, ^o R _V	17340.41 Z	(5)
X	$1\Sigma^+$	0	1604.52 Z	28.77 ^p	6.137 ^f	0.181 ^q	342 ^r	1.663 ₀			
$^{69}\text{Ga}^2\text{H}$											
		$(\mu = 1.95691832)$	$D_0^0 < 2.86 \text{ eV}^a$						JUL 1976		
A	1Π				[2.61] ^c		[100]	[1.82]	A \leftarrow X, R	23860.2 ^s Z	(6)
a	$3\Pi_1$				[3.339]		[113]	[1.606 ₂]	a \leftarrow X, V	17634.36 Z	(2)
X	$1\Sigma^+$	0			[3.083]	0.06 ₃	[84]	1.663 ₁			

- GaF: ^aThermochemical value (mass-spectrom.)(5).
^b $w_e v_e = -0.6_0$. This state may have a small potential maximum of ~ 0.26 eV (5).
^c $\gamma_e = -(0.0003)$. Rotational constants estimated from observed R-Q or P-Q head separations and B".
^d $w_e v_e = -0.43_3$.
^eRecalculated from (3) with the more accurate ground state constants of (6).
^f Λ -type doubling, $B_{RP} - B_Q \approx +6 \times 10^{-5}$.
^g $w_e v_e = -0.3_1$.
^h $\gamma_e = +0.0000102$.
ⁱ $\mu_{el}(v=0) = 2.45$ D (6);
 $eqQ(^{69}\text{Ga}) = -[107.07 - 1.09(v+\frac{1}{2})]$ MHz (6)(7),
 $g_J(v=0) = -0.0601_2 \mu_N$ (7).
 (1) Welti, Barrow, Nature 168, 161 (1951); PPS A 65, 629 (1952).
 (2) Barrow, Jacquest, Thompson, PPS A 67, 528 (1954).
 (3) Barrow, Dodsworth, Zeeman, PPS A 70, 34 (1957).
 (4) See ref. (3) of BaBr.
 (5) Murad, Hildenbrand, Main, JCP 45, 263 (1966).
 (6) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 1029 (1970).
 (7) Honerjäger, Tischer, ZN 29 a, 1919 (1974).

Ga¹H, Ga²H:

- ^aFrom the predissociation of A ¹ $\Pi(v=0)$, see ^c.
^bFrom the value for Ga²H.
^cDeuteride bands involving this level have diffuse rotational lines whose width increases with J. Corresponding lines of the hydride are even broader, only diffuse Q and R heads can be recognized. The diffuseness results from tunnelling through a potential maximum which separates the shallow potential well from the dissociation limit $^2P_{3/2} + ^2S$.

Ga¹H, Ga²H (continued):

- ^d $D_{RP} - D_Q = +12 \times 10^{-6}$.
^e $w_e y_e = -7.47$.
^fRKR potential functions (4).
^g $\gamma_e = -0.0315$. Rotational constants derived from R and P branches. Slightly different B_v and D_v values from the Q branches; see (3).
^h $-124 \times 10^{-6}(v+\frac{1}{2}) + 83.5 \times 10^{-6}(v+\frac{1}{2})^2$; see ^g.
ⁱ $w_e y_e = -6.195$.
^j $\gamma_e = -0.0400$.
^k $+75 \times 10^{-6}(v+\frac{1}{2}) + 14.5 \times 10^{-6}(v+\frac{1}{2})^2$.
^l $\Delta G(3/2) = 1313.6$.
^m $\gamma_e = -0.058$.
ⁿ $D_1 = 413 \times 10^{-6}$, $D_2 = 46_3 \times 10^{-6}$.
^oEach band consists of a single Q branch.
^p $w_e y_e = +0.360$.
^q $\gamma_e = -0.0005$.
^r $+1 \times 10^{-6}(v+\frac{1}{2})^2$.
^sCalculated from $v_0(0-1) = 22745.8$ using ground state vibrational constants derived from Ga¹H. The 0-0 band was not observed owing to a strong overlapping impurity.
 (1) Garton, PPS A 64, 509 (1951).
 (2) Neuhaus, Nature 180, 433 (1957); AF 14, 551 (1959).
 (3) Ginter, Innes, JMS 7, 64 (1961).
 (4) Ginter, Battino, JCP 42, 3222 (1965).
 (5) Poynor, Innes, Ginter, JMS 23, 237 (1967).
 (6) Kronekvist, Lagerqvist, Neuhaus, JMS 39, 516 (1971).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{69}\text{Ga}^{127}\text{I}$										
		$\mu = 44.666098_4$ $D_0^0 = 3.4_7 \text{ eV}^a$								SEP 1976
		Continuous absorption with maximum at 32600 cm^{-1} .								(1)
C 1Π								$C \leftarrow X,$		(1)
B $3\Pi_1$	25900.6	185.0	H ^Q	2.7				$B \leftrightarrow X,$ ^b 25884.3 H ^Q		(1)*
A $3\Pi_0^+$	25571.0	193.2	H	2.4				$A \leftrightarrow X,$ ^b 25559.0 H		(1)*
X $1\Sigma^+$	0	216.6	H ^Q	0.5	0.056934 ₇	0.000189	(0.157)	2.57467	Microwave sp. ^c	(2)
$^{69}\text{Ga}^{160}$										
		$(\mu = 12.9822464_3)$ $D_0^0 = 3.9_1 \text{ eV}^a$								SEP 1976
		Additional unclassified emission bands in the region $20000 - 23000 \text{ cm}^{-1}$.								(1)
B 2Σ	25706.9	762.9 ^b	H	3.44	[(0.4013)]	[(2.9)]	[(1.798 ₈)]	$B \leftrightarrow X,$ R 25705.3 H		(1)* (2)(4)
X 2Σ	0	767.5 ^b	H	6.24	[(0.4271)]	[(3.7)]	[(1.743 ₆)]			(5)
$^{69}\text{Ga}^{31}\text{P}$										
		$(\mu = 21.3703567)$ $D_0^0 = 2.3_8 \text{ eV}^a$								SEP 1976
$^{69}\text{Ga}^{(130)}\text{Te}$										
		$(\mu = 45.032342_9)$ $D_0^0 = 2.7_3 \text{ eV}^a$								SEP 1976
$^{69}\text{Ga}^{75}\text{As}$										
		$(\mu = 35.899311_5)$ $D_0^0 = 2.1_8 \text{ eV}^a$								SEP 1976
$^{69}\text{Ga}^{209}\text{Bi}$										
		$(\mu = 51.830821_4)$ $D_0^0 = 1.6_0 \text{ eV}^a$								SEP 1976

GaI: ^aExtrapolation of vibrational intervals in A and B; see the discussion in (3).

^bBoth directions of shading occur, even in one and the same band.

^ceqQ(⁶⁹Ga) = - 66 MHz,

eqQ(¹²⁷I) = - 549 MHz.

(1) See ref. (1) of GaBr.

(2) See ref. (2) of GaBr.

(3) See ref. (3) of GaBr.

GaO: ^aThermochemical value (mass-spectrom.)(6). For flame photometric results see (3)(4).

^bConstants from (5) who attribute the double heads observed for most bands to isotope splitting; (1) assumes spin doubling. (1), (2), and (4) give all slightly different constants.

(1) Guernsey, PR 46, 114 (1934).

(2) Sen, IJP 10, 429 (1936).

(3) Gurvich, Velts, BASPS 22, 670 (1958).

(4) Gurvich, Novikov, Ryabova, OS(Engl. Transl.) 18, 68 (1965).

(5) Raziunas, Macur, Katz, JCP 39, 1161 (1963); 42, 2634 (1965).

(6) Burns, JCP 44, 3307 (1966).

GaP: ^aThermochemical value (mass-spectrom.)(1)(2).

(1) Gingerich, Piacente, JCP 54, 2498 (1971).

(2) Piacente, Gingerich, HTS 3, 219 (1971).

GaTe: ^aThermochemical value (mass-spectrom.)(1), adjusted to the new value of D₀⁰(Te₂); see DONNSPEC (1970).

(1) Uy, Muenow, Ficalora, Margrave, TFS 64, 2998 (1968).

GaAs: ^aThermochemical value (mass-spectrom.)(1).

(1) De Maria, Malaspina, Piacente, JCP 52, 1019 (1970).

GaBi: ^aThermochemical value (mass-spectrom.)(1).

(1) Piacente, Desideri, JCP 57, 2213 (1972).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(^{158})\text{Gd}^{19}\text{F}$		$(\mu = 16.9583061)$		$D_0^0 = (6.0_8) \text{ eV}^a$						JAN 1975
$(^{158})\text{Gd}^{16}\text{O}$		$(\mu = 14.5239012_1)$		$D_0^0 = 7.3_7 \text{ eV}^a$						JAN 1975 A
		Large number of mostly R shaded bands in emission from 13300 to 22500 cm^{-1} . Two systems of bands with multiple heads were identified by (1) and confirmed and extended by (4)(7):								(2)* (4)*
System I:		$\nu_H = 21700.5 + 748.0(\nu' + \frac{1}{2}) - 3.0(\nu' + \frac{1}{2})^2 - 830.1(\nu'' + \frac{1}{2}) + 2.3(\nu'' + \frac{1}{2})^2$						R 21659.3	H	(1)(4)(7)
System II:		$\nu_H = 20470.5 + 767.0(\nu' + \frac{1}{2}) - 4.9(\nu' + \frac{1}{2})^2 - 836.0(\nu'' + \frac{1}{2}) + 2.8(\nu'' + \frac{1}{2})^2$						R 20435.5	H	
		Assignments at longer wavelengths are less certain, and considerable disagreement exists between analyses by (1)(3)(7) except in the region 15700 - 16200 cm^{-1} where three long sequences have been identified:						R 16170 R 16122 R 16094	H H H	(1)(3)(7)
$(^{158})\text{Gd}^{(32)}\text{S}$		$(\mu = 26.5890611)$		$D_0^0 = 5.3_7 \text{ eV}^a$						JAN 1975
$(^{158})\text{Gd}^{(80)}\text{Se}$		$(\mu = 53.063878_1)$		$D_0^0 = 4.4_1 \text{ eV}^a$						JAN 1975
$(^{158})\text{Gd}^{(130)}\text{Te}$		$(\mu = 71.275762)$		$D_0^0 = 3.4_9 \text{ eV}^a$						JAN 1975
$(^{72,74})\text{Ge}_2$		$(\mu = 36.4539647)$		$D_0^0 = 2.8_2 \text{ eV}^a$						SEP 1976

GdF: ^aThermochemical value (mass-spectrom.), quoted from (1).
Re-evaluation using the reaction enthalpies and auxiliary data in (1) results, however, in 6.9₅ eV.
(1) Zmbov, Margrave, JINC 29, 59 (1967).

GdO: ^aThermochemical value (mass-spectrom.)(5)(6)(8).
(1) Piccardi, GCI 63, 887 (1933).
(2) Gatterer, RS 1, 153 (1942).
(3) Lemaitre, Rosen, quoted in (4).
(4) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
(5) Ames, Walsh, White, JPC 71, 2707 (1967).
(6) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).
(7) Suárez, Grinfeld, JCP 53, 1110 (1970).
(8) Drowart, Myers, Szwarc, Vander Auwera-Mahieu, Uy, to be published.

GdS: ^aThermochemical value (mass-spectrom.)(1), recalcd. (2).
(1) See ref. (6) of GdO.
(2) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

GdSe, GdTe:
^aThermochemical value (mass-spectrom.)(1).
(1) See ref. (2) of GdS.

Ge₂: ^aThermochemical value (mass-spectrom.)(1).
(1) Kant, JCP 44, 2450 (1966).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(⁷⁴Ge(⁷⁹Br		$(\mu = 38.1690316) \quad D_0^0 = (3.5) \text{ eV}^a$ Additional unassigned absorption bands above 43000 cm^{-1} .								SEP 1976
G	47544	358	H	1.5				$G \leftarrow X$, V	$\overline{47577}$ H	(6)*
F								$F \leftarrow X$, V	$\overline{45946}$ H	(6)*
E ($^2\Sigma^+$)	44805	366	H	5				$E \leftarrow X$, V	$\overline{43689}$ H $\overline{44840}$ H	(6)*
D	^c							$D \leftarrow X$, V	$\overline{43296}$ H $\overline{44426}$ H	(6)*
C ($^2\Pi$)	(41156) 41046	359	H	3				$C \leftarrow X$, V	(40037) $\overline{41077}$ H	(6)*
B ($^2\Sigma^+$)	33413	383.7	H	0.7				$B \leftrightarrow X$, V	$\overline{32307}$ H $\overline{33457}$ H	(1)* (6)
A' ($^2\Delta$)	27252 27156	197.3 190.1	H H	7.2 7.3				$A' \rightarrow X$, R	26051.5 H 27102.1 H	(2)*
A ($^2\Sigma$)		Bands in the region $17000 - 23000 \text{ cm}^{-1}$. Different vibrational analyses, $\omega_e' \approx 190$.						$A \rightarrow X$, R		(3)(4)(5)
X $^2\Pi_r$	1150 0	295.4	H	0.7 ₂						
(⁷⁴Ge¹²C		$(\mu = 10.32404534) \quad D_0^0 = 4.7_3 \text{ eV}^a$								SEP 1976
⁷⁴Ge³⁵Cl		$\mu = 23.7389853 \quad D_0^0 = (4.4) \text{ eV}^a$ Tentative assignments of bands above 46000 cm^{-1} .								SEP 1976
(D)								$(D \leftarrow X)$,	$\overline{46640}$ H $\overline{47586}$ H	(7)
C ($^2\Pi$)	45845 45824	493.4	H	2.0				$C \leftarrow X$, V	$\overline{44914}$ H $\overline{45867}$ H	(7)*
C'	42181	506.9	H	3.7				$C' \leftarrow X$, V	$\overline{42230}$ H	(7)*
B ($^2\Sigma$)	33992.2	526.6 ^b	H	(0.3)				$B \leftrightarrow X$, V	33078.0 H $\overline{34052.0}$ H	(1)* (2)(4) (7)*

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{74}\text{Ge}^{35}\text{Cl}$ (continued)											
$A'(^2\Delta_r)$	29561.7 29499.8	335.5 342.1	H H	4.58 4.65				$A' \rightarrow X,^d$ R	28550.9 29466.2	H H	(2)*
$A(^2\Sigma^+)$		Bands in the region 16000 - 25000 cm^{-1} . Different vibrational analyses, $w_e' \approx 250$.						$A \rightarrow X,$ R			(3)(5)
$X^2\Pi_r$	975.0 0	405.5 407.6	H H	1.23 1.36	c						

GeBr: ^aExtrapolation of vibrational levels in A' ; atomic products at the limit uncertain.

^bIt is possible that more than one transition is involved.

^cDoublet separation $\approx 20 \text{ cm}^{-1}$.

- (1) Jevons, Bahford, Briscoe, PPS 49, 532 (1937).
- (2) Andrews, Barrow, PPS A 63, 957 (1950).
- (3) Kuznetsova, Kuzyakov, IVUZK 12 (9), 1183 (1969).
- (4) Rao, Haranath, JP B 2, 1385 (1969).
- (5) Chatalic, Deschamps, Pannetier, JCPPB 67, 335 (1970).
- (6) Oldershaw, Robinson, TFS 67, 2499 (1971).

GeC: ^aThermochemical value (mass-spectrom.)(1).

- (1) Drowart, De Maria, Boerboom, Inghram, JCP 30, 308 (1959).

GeCl: ^aSee ^a of GeBr.

^b(4) and (6) give slightly different constants.

^cPartial rotational analysis of two subbands (6).

^dThe bands have at least two heads of comparable intensity.

- (1) See ref. (1) of GeBr.
- (2) Barrow, Lagerqvist, AF 1, 221 (1949).
- (3) Deschamps, Robert, Pannetier, JCPPB 65, 1084 (1968).
- (4) Filippova, Kuzyakov, VMUK No. 3, 25 (1968).
- (5) Rao, Haranath, JP B 2, 1080 (1969).
- (6) Mishra, Khanna, IJPAP 8, 825 (1970).
- (7) Oldershaw, Robinson, TFS 66, 532 (1970).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{74}\text{Ge}^{19}\text{F}$		$\mu = 15.1139772$	$D_0^0 = 5.0_0 \text{ eV}^a$		$\text{I.P.} = 7.4_6 \text{ eV}^b$					SEP 1976	
G $^2\Delta_r(4d\delta)$ 49412.89 ^c	[710.37]	Z	2.82	H	0.38408	0.00261	[4.43] ^d	1.7041 ₁	G \rightarrow X, V	48523.4 H ^Q 49415.6 H ^Q	(2)(7)*
D $^2\Sigma^+(6s\sigma)$ 48581.26	833.12	Z ^e	6.52	H	0.39972 ^e	0.00214	[3.73] ^f	1.6704	D \rightarrow A, V	25473.3 ₀ Z	(7)*
									D \rightarrow X, V	47726.6 H ^Q 48662.6 H ^Q	(7)*
D' $^2\Pi(4d\pi)$ 47920.73 ^g	803.96 ^h	Z	3.38	H	0.40068 ^{hi}	0.00259	3.6 ₂ ^h	1.6684	D' \rightarrow A, V	24798.9 ₈ H ^h Z	(7)*
									D' \rightarrow X, ^j V	47043.0 H 47976.3 H	(7)*
E $^2\Sigma^+(5p\sigma)$ 46645.41	760.08	Z	2.967		0.39845 ^k	0.00290	4.33	1.6731 ₀	E \rightarrow B, ^l	11616.26 Z	(7)*
C $^2\Delta$ 43977.49 ^m	[684.00]	Z	9.31		0.38835	0.00421	[4.97] ⁿ	1.6947 ₂	C \rightarrow X, V	43059.27 ^o Z 43994.43 ^o Z	(2)(4)(7)*
C' $^2\Pi(5p\pi)$ 43369.61 ^p	796.88	Z	3.415		0.39957 ^q	0.00258	4.13	1.6707 ₅	C' \rightarrow A, ^r R	20244.31	(7)
									C' \rightarrow X, ^s V	42547.8 H 43377.9 H	(4)(7)*
a $^4\Sigma^-$ 35194.68 ^t	[628.31]	Z	6.66 ^u		0.36676 ^t	0.00369	[4.94] ^v	1.7439	a \rightarrow X,	35181.77 Z	(6)*
B $^2\Sigma^+(5s\sigma)$ 35010.85	796.99	Z	3.613 ^w		0.39440 ^x	0.00255	3.88	1.6816 ₇	B \rightarrow A, V	11885.56 Z	(2)
									B \rightarrow X, ^y V	34141.23 Z 35076.39 Z	(1)* (6)*
A $^2\Sigma^+$ 23316.65	413.03	Z	1.124 ^z		0.32039 ^{a'}	0.00307 ^{b'}	7.78 ^{c'}	1.8658 ₂	A \rightarrow X, ^y R	22255.67 Z 23190.83 Z	(1)* (6)*
X $^2\Pi_{3/2}$ 934.33	667.33	Z			0.36660	0.00267 ^{f'}	4.50	1.7452			
$^2\Pi_{1/2}$ 0	665.67	Z			0.36578 ^{e'}		4.47				

GeF: ^aThermochemical value (mass-spectrom.) (3); see also (5).
^bApproximate limit of the ns (n = 5, 6, ...) Rydberg series (7). (5) give 7.2 eV from electron impact mass-spectrometry.
^c $A_0 = +22.20$, $A_1 = +21.5$; small J dependence.
^d $D_1 = 4.52 \times 10^{-7}$.
^eRotational analysis of v=2, and tentative results for v=0.
^f $D_2 = 3.33 \times 10^{-7}$.
^g $A_2 = (+)4.23$, $A_3 = (+)4.35$.
^hExtrapolation from the rotationally analyzed levels v'=2 and 3; $\beta_e = +0.21 \times 10^{-7}$.
ⁱLarge Λ -type doubling, also spin-rotation interaction; see (7).
^jThe 0-1 and 0-2 bands were previously considered by (2) as 0-0 bands of their transitions F-X and E-X, resp..
^kSpin-doubling constant $\gamma(v=0) = -0.0358$.
^l $\Delta v=0$ sequence of slightly V shaded bands, provisionally assigned in (2) to a $E(^2\Pi) - B(^2\Sigma)$ transition.
^m $A_0 = 13.88$, $A_1 = 14.25$.
ⁿ $D_1 = 5.15 \times 10^{-7}$.
^oReferring in the upper state to the zero point of the Hill - Van Vleck expression.
^p $A_0 = 105.63$, $A_1 = 105.88$, $A_2 = 105.96$; small J dependence.
^q Λ -type doubling in $^2\Pi_{1/2}$, $\Delta v_{fe}(v=0) = -0.0373(J+\frac{1}{2})$.
^rExtremely weak system consisting of a long 0-v" progression; not analyzed.
^sThe 3-1 and 1-0 bands of $C \cdot ^2\Pi_{1/2} - X^2\Pi_{1/2}$ correspond to the 0-0 subbands of a system D-X proposed earlier by (2). The 2-1 band of the $3/2-3/2$ system was assigned by (2) as 0-0 band of $C' - X^2\Pi_{1/2}$.

^tSpin-splitting constants for v=0: $\lambda = +8.086$ [$4\lambda = T_0(^4\Sigma_{3/2}) - T_0(^4\Sigma_{1/2})$], $\gamma_1 \approx \gamma_2 = 0.0119$. See also ^x.
^uBased on the interpretation of a perturbation in $B^2\Sigma^+$, v=4.
^v $D_1 = 4.90 \times 10^{-7}$.
^w $w_{ey_e} = +0.0124$.
^xSpin-doubling constant $\gamma(v=0) = +0.00100$. Extensive perturbations between $B^2\Sigma^+$, v=0 and $a^4\Sigma^-$, v=0.
^yFranck-Condon factors (8).
^z $w_{ey_e} = -0.0129$.
^aSpin-doubling constant $\gamma(v) = -[0.03662 + 0.00014(v+\frac{1}{2})]$.
^b $\gamma_e = +0.000038$.
^c $-0.22 \times 10^{-7}(v+\frac{1}{2}) + \dots$
^d $w_{ey_e} = +0.0068$.
^e Λ -type doubling, $\Delta v_{fe} = -[0.0218_4 + 0.00019_5(v+\frac{1}{2})](J+\frac{1}{2})$.
^f $\gamma_e = +0.000008_3$.
(1) Andrews, Barrow, PPS A 63, 185 (1950).
(2) Barrow, Butler, Johns, Powell, PPS 23, 317 (1959).
(3) Ehler, Margrave, JCP 41, 1066 (1964).
(4) Uzikov, Kuzyakov, VMUK No. 5, 30 (1969).
(5) Harland, Cradock, Thynne, INCL 2, 53 (1973).
(6) Martin, Merer, CJP 51, 125 (1973).
(7) Martin, Merer, CJP 52, 1458 (1974).
(8) Singh, IJPAP 13, 204 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{72}\text{Ge}^1\text{H}$		$\mu = 0.99389799$ $D_0^0 \leq 3.3 \text{ eV}^a$								SEP 1976
B ($^2\Sigma$)	[41074]	Incompletely resolved bands.						B \leftarrow X, R	39686 40573	H H (3)
A $^2\Delta$	25454 ^b	[1185.15]	Z (127) ^c	6.535 ^d	0.619 ₆	[5.71] ^e	1.611	A \leftrightarrow X, R	25197.0	Z (1)* (6)* (9)
a $^4\Sigma(-)$	[16747] ^f			[6.7654] ^f		[4.60]	[1.5834]	a \rightarrow X, V	15802.8	Z (2)(5)
X $^2\Pi_r$	0 ^g	[1833.77]	Z (37) ^c	6.725 ₉ ^h	0.191 ₆	[3.26] ⁱ	1.5880			
$^{72}\text{Ge}^2\text{H}$		$\mu = 1.95923588$ $D_0^0 \leq 3.3 \text{ eV}^j$								SEP 1976
A $^2\Delta$	25460 ^k	1027.82	Z 65.73	3.286 ₀ ^l	0.167 ₀ ^m	[1.40] ⁿ	1.6182	A \leftrightarrow X, R	25283.0	Z (6)* (9)
X $^2\Pi_r$	0 ^o	[1320.09]	Z (19) ^c	3.414 ₅ ^p	0.070 ₂	[0.832] ^q	1.5874			
$^{74}\text{Ge}^{127}\text{I}$		$\mu = 46.711803_0$								SEP 1976
		Additional absorption bands above 40000 cm^{-1} ; tentative assignments.								(3)
G								G \leftarrow X ₁ , ^a V	43959	(4)*
F	42769	292	H 2					F \leftarrow X ₂ , ^a V	41376	
E								F \leftarrow X ₁ , ^a V	42792	H (3)(4)*
D								E \leftarrow X ₁ , ^a V	42639	(4)*
C								D \leftarrow X ₁ , ^a V	41781	(3)(4)*
								C \leftarrow X ₁ , ^a V	41404	(3)(4)*
B ($^2\Sigma$)	32650.1	305.9 ^b	H 0.67					B \leftarrow X ₂ , fragments only.		(2)
A ($^2\Sigma$)	18663	155.2	H 0.58					B \leftarrow X ₁ , ^a V	32679.9	H (1)* (2)
X ₂ $^2\Pi_{3/2}$	(1413)							A \rightarrow X ₁ , R	18617	H (2)
X ₁ $^2\Pi_{1/2}$	0	246.3	H 0.75							

Ge¹H, Ge²H:

- ^aFrom the predissociation in A ²Δ (6); thermochemical data give the same value (4).
^bA₀ = 10.3, A₁ = 6.1; moderate J dependence. For a more detailed theoretical discussion of this ²Δ state see (8).
^cEstimated from isotope shifts (6).
^dSpin-doubling constants γ = 0.473 (v=0) and 0.362 (v=1). Broadening of absorption lines due to predissociation above 27000 cm⁻¹.
^eD₁ = 8.01 x 10⁻⁴; also higher order constants.
^fSpin-splitting constants λ = 6.52, γ₁ = 0.037, γ₂ = 0.048. Note, that the definitions of λ, γ₁, and γ₂ used in (5) are those of Hougen (4a) and differ from those used by Martin and Merer [see ref. (6) of GeF]. The B₀ value in the abstract of (5) and quoted in DONNSPEC is clearly wrong.
^gA₀ = 892.52, A₁ = 896.12 from (6); small J dependence. See also (9).
^hΛ-type doubling; in ²Π_{1/2}(v=0), Δv = 0.496(J+½) - ...
ⁱD₁ = 3.40 x 10⁻⁴.
^jFrom the value for Ge¹H.
^kA₀ = 14.4, A₁ = 9.9, A₂ = 7.2; moderate J dependence.
^lSpin-doubling constants γ = 0.300 (v=0), 0.281 (v=1), 0.22 (v=2). Predissociation, see ^d.
^mγ_e = - 0.021₉.
ⁿD₁ = 1.65 x 10⁻⁴, D₂ = 1.7 x 10⁻⁴; also higher order constants.

Ge¹H, Ge²H (continued):

- ^oA₀ = 891.86, A₁ = 894.35 from (6); small J dependence. See also (9).
^pΛ-type doubling; in ²Π_{1/2}(v=0), Δv = 0.2506(J+½) - ...
^qD₁ = 0.824 x 10⁻⁴.
 (1) Kleman, Werhagen, AF 6, 359 (1953).
 (2) Kleman, Werhagen, AF 6, 399 (1953).
 (3) Barrow, Drummond, Garton, PPS A 66, 191 (1953).
 (4) Barrow, Deutsch, PCS (1960), 122.
 (4a) Hougen, CJP 40, 598 (1962).
 (5) Klynning, AF 32, 563 (1966).
 (6) Klynning, Lindgren, AF 32, 575 (1966).
 (7) Kovács, Pacher, JP B 4, 1633 (1971).
 (8) Veseth, Physica 56, 286 (1971).
 (9) Veseth, JMS 48, 283 (1973).

- GeI: ^aThe systems B-X, C-X, D-X, F-X, and G-X of (1)(4) correspond to C-X, D-X, E-X, F-X, and H-X of (2)(3).
^bVibrational numbering of (2), based on observed isotope shifts and confirmed by (4).
 (1) Oldershaw, Robinson, TFS 64, 2256 (1968).
 (2) Chatalic, Deschamps, Pannetier, JCPBP 67, 1567 (1970).
 (3) Chatalic, Iacocca, Pannetier, CR C 274, 1784 (1972).
 (4) Oldershaw, Robinson, JMS 44, 602 (1972).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{74}\text{Ge}^{16}\text{O}$		$\mu = 13.1496256_4$ $D_0^0 = 6.78 \text{ eV}^a$ I.P. = 11.1_0 eV^b Additional unassigned R shaded absorption bands between 66800 and 69900 cm^{-1} .								SEP 1976 A
F	67474.5	809.0	H 5.66					F \leftarrow X, R	67390 H	(3)*
E	49637.3	504.3	H 4.8					E \leftrightarrow X, R	49397 H	(3)* (16)*
A $^1\Pi$	37766.9 H	650.4	H 4.21	0.413_3^{cd}	0.0033	8.2	1.761	A \leftrightarrow X, ^d R	37595.4 Z	(1)* (2)* (8)* (13) (16)(18)*
a ($^3\Pi_1$)	32132	734.9	H 5.3	(0.438)			(1.71 ₁)	a \rightarrow X, ^d R	32007 H	(7)(25)*
a' ($^3\Sigma^+$)	27733	633.3	H 2.7	(0.389)			(1.81 ₅)	a' \rightarrow X, ^{de} R	27553 H	(21)(24)* (25)*
(B)	(21117)	(580.0)	H (3.5)	Observed in thermal emission. ^f				(B \rightarrow X), R	(20917)	(15)
X $^1\Sigma^+$	0	985.5 ^g	H 4.29 ^g	0.4856962^d	0.0030756	4.72 ^h	1.624648	Microwave sp. Mol. beam el. reson. ^{ij}		(6)(9)(17) (10)(20)
$^{74}\text{Ge}^{32}\text{S}$		$\mu = 22.3188284$ $D_0^0 = 5.67 \text{ eV}^a$								SEP 1976
E	38884.8	310.3	H 1.43 ^b					E \leftarrow X, R	38752.1 H	(1)(3)*
A $^1\Pi$	32889.5	375.0	H 1.51					A \leftrightarrow X, R	32789.2 H	(1)(2)* (3)*
a ($^3\Pi$)								a \rightarrow X,	(22400) ^c	(8)
X $^1\Sigma^+$	0	575.8	H 1.80	0.18656575_7	0.00074910_3^d	0.7883^e	2.012086^f	IR sp. ^g Microwave sp. ^h		(9) (5)(10)

GeO: a Thermochemical value (mass-spectrom.)(4).

b Vertical I.P. from electron impact mass spectrometry (12).

c Perturbation between A $^1\Pi(v=0)$ and a $^3\Pi(v=8)$, see (25).

d RKR potential curves (5)(22), Franck-Condon factors (19)(23)(25); variation of A-X electronic transition moment (26).

GeO (continued):

e Also observed in phosphorescence in various solid matrices at low temperature (14); lifetime in matrices (11).

f The vibrational analysis seems uncertain since the intensity distribution does not agree with that expected for such a large change of ω_e .

GeO (continued):

^gFrom band origins (13) obtain $\omega_e = 986.84$, $\omega_e x_e = 4.47$.

^hCalculated D_e .

ⁱ $\mu_{el}(^+GeO^-) = [3.2720 + 0.0208(v+\frac{1}{2})] D$ (10).

^j $g_J(v=0) = -0.1411$ (17)(20); also magnetic susceptibility anisotropy and molecular quadrupole moment.

(1) Jevons, Bashford, Briscoe, PPS 49, 543 (1937).

(2) Drummond, Barrow, PPS A 65, 277 (1952).

(3) Barrow, Rowlinson, PRS A 224, 374 (1954).

(4) Drowart, Degreè, Verhaegen, Colin, TFS 61, 1072 (1965).

(5) Nair, Singh, Rai, JCP 43, 3570 (1965); IJPAP 2, 130 (1971).

(6) Törring, ZN 21 a, 287 (1966).

(7) Sharma, Padur, PPS 90, 269 (1967).

(8) Majumdar, Mohan, IJPAP 6, 183 (1968).

(9) Hoeft, Lovas, Tiemann, Tischer, Törring, ZN 24 a, 1217 (1969).

(10) Raymonda, Muentner, Klemperer, JCP 52, 3458 (1970).

(11) Meyer, Smith, Spitzer, JCP 53, 3616 (1970).

(12) Hildenbrand, IJMSIP 7, 255 (1971).

(13) Korzh, Kuznetsova, OS(Engl. Transl.) 31, 286 (1971).

(14) Meyer, Jones, Smith, Spitzer, JMS 37, 100 (1971).

(15) Tewari, Mohan, JMS 39, 290 (1971).

(16) Murty, Reddy, Rao, IJPAP 10, 834 (1972).

(17) Honerjäger, Tischer, ZN 28 a, 1374 (1973).

(18) Murty, Rao, Rao, PRIA A 73, 213 (1973).

(19) Sinha, Chatterjee, IJPAP 11, 57 (1973).

(20) Davis, Muentner, JCP 61, 2940 (1974).

(21) Hager, Wilson, Hadley, CPL 27, 439 (1974).

(22) Savithry, Rao, Rao, CS 43, 329 (1974).

(23) Singh, IJPAP 12, 528 (1974).

(24) Hager, Harris, Hadley, JCP 63, 2810 (1975).

(25) Capelle, Brom, JCP 63, 5168 (1975).

(26) Rao, Rao, Rao, JQSRT 16, 467 (1976).

GeS: ^aThermochemical value (mass-spectrom.) (4). The convergence limit in E-X, assuming dissociation into $^3P + ^3P$, gives 5.66 ± 0.13 eV, the error being due to the uncertainty with regard to the particular triplet components involved.

^bExtended progression ($v''=0$) converging to 46715 cm^{-1} . The vibrational constants given represent this progression up to $v'=17$ only.

^cExtrapolated from observed phosphorescence spectra in various solid matrices at low temperature (8). Lifetime in these matrices (7).

^d $-4.4 \times 10^{-8}(v+\frac{1}{2})^2 - 2.8 \times 10^{-9}(v+\frac{1}{2})^3$.

^e $\beta_e = +0.0010 \times 10^{-7}$.

^fFrom the effective B_e ; 2.012043 Å at the minimum of the Born-Oppenheimer potential curve, see (10).

^gIn low-temperature argon and nitrogen matrices.

^h $\mu_{el}(v=0) = 2.00 D$ from Stark effect of microwave spectrum (5). Quadrupole hyperfine structure for isotopic molecules with nuclear spins $I \geq 1$ (6).

(1) Shapiro, Gibbs, Laubengayer, PR 40, 354 (1932).

(2) Barrow, PPS 53, 116 (1941).

(3) See ref. (2) of GeO.

(4) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).

(5) See ref. (9) of GeO.

(6) Hoeft, Lovas, Tiemann, Törring, JCP 53, 2736 (1970).

(7) See ref. (11) of GeO.

(8) See ref. (14) of GeO.

(9) Marino, Guérin, Nixon, JMS 51, 160 (1974).

(10) Stieda, Tiemann, Törring, Hoeft, ZN 31 a, 374 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{74}\text{Ge}^{80}\text{Se}$										
		$\mu = 38.401013_5$			$D_0^0 = 4.9_8 \text{ eV}^a$					SEP 1976
E	35462.6	217.7	H	1.02 ^b				E \leftarrow X, R	35367 H	(2)*
A $^1\Pi$	30845.7	269.4	H	0.89				A \leftrightarrow X, R	30776.2 H	(1)* (2)*
X $^1\Sigma^+$	0	408.7	H	1.36	0.096340508	0.000289040 ^c	2.207 ₁ ^d	2.134629 ^e	IR sp. ^f Microwave sp. ^g	(6) (3)(7)
$(^{74})\text{Ge}^{(28)}\text{Si}$										
		$(\mu = 20.2956423)$			$D_0^0 = 3.0_8 \text{ eV}^a$					SEP 1976
$^{74}\text{Ge}^{130}\text{Te}$										
		$\mu = 47.112514_2$			$D_0^0 = 4.2_4 \text{ eV}^a$					SEP 1976
E	(31470)	(170)	H	(1.2)				E \leftarrow X, R	$\begin{smallmatrix} 31458 \\ 31401 \end{smallmatrix}$ ^b H H	(2)
A $^1\Pi$	27750.8	221.0	H	0.89				A \leftrightarrow X, R	27699.3 H	(1)* (2)
X $^1\Sigma^+$	0	323.9	H	0.75	0.06533821	0.00017246 ^c	1.1 ₈	2.340165	IR sp. ^d Microwave sp. ^e	(8) (4)

GeSe: ^aFrom the convergence of the E-X, v''=0 progression assuming dissociation into ³P+³P. Since the particular triplet components involved are uncertain the possible error is rather large, viz. ± 0.25 eV.
^bLong progression of absorption bands converging at 42360 cm⁻¹. The vibrational constants represent the levels only to v'=14.
^c $-3.4 \times 10^{-8}(v+\frac{1}{2})^2 - 1.1 \times 10^{-9}(v+\frac{1}{2})^3$.
^d $\beta_e = +0.0019 \times 10^{-8}$.
^eFrom the effective B_e. According to (7) the minimum of the Born-Oppenheimer potential curve is at 2.134603 Å.
^fIn low-temperature argon and nitrogen matrices.
 $\epsilon_{u_{el}}(v=0) = 1.64_8$ D from Stark effect of microwave spectrum (4). Hyperfine structure for odd isotopes (5).
 (1) Barrow, Jevons, PPS 52, 534 (1940).
 (2) See ref. (2) of GeO.
 (3) Hoeft, ZN 21 a, 1240 (1966).
 (4) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 539 (1970).
 (5) See ref. (6) of GeS.
 (6) See ref. (9) of GeS.
 (7) See ref. (10) of GeS.

GeSi: ^aThermochemical value (mass-spectrom.)(1).
 (1) See ref. (1) of GeC.
 GeTe: ^aThermochemical value (mass-spectrom.)(3), corrected for the new value of D₀⁰(Te₂). Extrapolation of the vibrational levels of the E state (2) gives 4.1 \pm 0.4 eV.
^bThere seem to be two components of this band system, possibly owing to strong perturbations.
^c $\gamma_e = -5.0 \times 10^{-8}$.
^dIn low-temperature nitrogen matrix.
^e $\mu_{el}(v=0) = 1.06$ D from Stark effect of microwave spectrum (5); hyperfine structure of ⁷³Ge (7). See also (6).
 (1) See ref. (1) of GeSe.
 (2) See ref. (2) of GeO.
 (3) Colin, Drowart, JPC 68, 428 (1964).
 (4) Hoeft, Nolting, ZN 22 a, 1121 (1967).
 (5) See ref. (4) of GeSe.
 (6) See ref. (6) of GeS.
 (7) Tiemann, Hoeft, Törring, ZN 26 a, 1930 (1971).
 (8) See ref. (9) of GeS.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^1\text{H}_2$		$\mu = 0.50391261$ $D_0^0 = 4.4781_3 \text{ eV}^a$ I.P. = 15.4258_9 eV^b							NOV 1976 A	
		WAVELENGTH TABLES of the H_2 spectrum from 2800 to 29000 \AA with assignments of many of the lines (109). The TABLES OF ENERGY LEVELS (24) are also very useful as long as it is realized that the absolute values of the energy levels ($n \geq 2$) relative to the ground state need correction. Graphs and tables of POTENTIAL ENERGY CURVES for all known states of H_2 , H_2^+ , and H_2^- (107).								
		Fragments of three other triplet systems. ^c								
u $^3\Pi_u$ 6p π [123488.0]		Only $v=0$ observed.		[29.3]		[2.3]	[1.06 ₉]	u \rightarrow a, δ bands	26232.3 ^f	(1)(24)
t ^d $^3\Sigma_u^+$ 5f σ (121292)		(2661.4)	(121.9)	e				t \rightarrow a,	(25342)	(4)
q ^d ($^3\Sigma_g^+$) 5d σ (121295)		[2172.6]		e				q \rightarrow c,	(25325) ^f	(3)
n $^3\Pi_u$ 5p π 120952.9		2321.4	62.8 ₆	29.9 ₅	1.24 ^g	[2.3]	1.057	n \rightarrow a, γ bands	24847.3 ^f	(1)(24)
m ^h $^3\Sigma_u^+$ 4f σ (119317)		[2457.1]		e				m \rightarrow a,	23295.1 ⁱ	(4)
s $^3\Delta_g$ 4d δ 118875.2		2291.7 ^j	62.4 ₄ ^j	k				s \rightarrow c,	22949.3 ^l	(1)(18)(24)
r $^3\Pi_g$ 4d π 118613.7		2280.3 ^m	57.9 ₆ ^m	k				r \rightarrow c,	22683.2 ^m	(1)(18)(24)
p $^3\Sigma_g^+$ 4d σ 118509.8		2303.1	76.9 ₀	e				p \rightarrow k, ⁿ		(154)
v ($^3\Pi_g$) ^o (118330)		(2340)	(57)	([29.1])			([1.07 ₂])	p \rightarrow c,	22586.0 ^f	(1)(18)(24)
k $^3\Pi_u$ 4p π 118366.2 ^p		2344.37	67.2 ₉ ^q	30.07 ₄	1.46 ₂ ^r	[1.8 ₅]	1.054 ₇	v \rightarrow c,	(22430)	(3)
f $^3\Sigma_u^+$ 4p σ (116705)		[2143.6] ^s		[27.0] ^s			[1.11]	k \rightarrow a, β bands	22271.0 ^f	(1)(15a)(24)
o ^t $^3\Sigma_u^+$ (114234)		2399.1	91.0	[35]			[0.98]	f \rightarrow a,	20526.0 ^s	(1)(24)
l ^u $^3\Pi_u$ 113825		2596.8	106.0	[36]			[0.96]	o \rightarrow a,	(18160)	(4)
								l \rightarrow a,	17846 ^f	(4)

See ^v p. 241

- ¹H₂: ^aThis is an upper limit ($36118.3 \pm 0.5 \text{ cm}^{-1}$), the lower limit being 4.4779 eV. According to (95) the true value is probably close to the upper limit; see also (101) who gives $D_0^0 = 36118.6 \text{ cm}^{-1}$ on the basis of a reassignment of the last vibrational levels of the B state. The most recent theoretical value of (70) - including a small non-adiabatic correction of (161) - is 36117.9 cm^{-1} . An earlier independent calculation (54) (not including the non-adiabatic correction) gave 36118.1 cm^{-1} .
- ^bFrom the limit of the np δ , $1\Sigma_u^+$ Rydberg series (124417.2 cm^{-1}) taking account of perturbations and pressure shift of high n lines (114). The earlier value of (98) was higher by 1.2 cm^{-1} because it was not corrected for pressure shift. The latest theoretical (ab initio) value (79) including relativistic, Lamb shift, and non-adiabatic corrections is 15.4259_0 eV ; see (114).
- ^c $3B \rightarrow c$, $3C \rightarrow c$, $7p\pi \rightarrow a$ (1)(3).
- ^dt and q are designated $3F$ and $3G$, resp., in (3)(4).
- ^eThe states $g^3\Sigma_g^+(3d\delta)$, $p^3\Sigma_g^+(4d\delta)$, $q^3\Sigma_g^+(5d\delta)$, $m^3\Sigma_u^+(4f\delta)$ and $t^3\Sigma_u^+(5f\delta)$ are strongly affected by ℓ -uncoupling. The N=1 levels lie below N=0 for v=0 and 1; meaningful B values cannot be given until the whole d and f complexes have been fully analysed, see (58).
- ^fReferred to the (non-existent) N=0 level in 3Π states; the N=1 levels of $c^3\Pi$ (+ and -) lie 60.7 cm^{-1} above N=0.
- ^gRepresents B_0 and B_1 of $3\Pi^-$ only; (4) gives $B_2 = 26.26$, $B_3 = 24.54$.
- ^h $3E$ of (4).
- ⁱRefers to N'=0 which lies above N'=4 because of strong ℓ -uncoupling.
- ^jConstants refer to N=2; from v=0, 1, 2.
- ^kBecause of strong ℓ -uncoupling no meaningful B values can be given; see ^e.
- ^lRefers to the N=2 level of $s^3\Delta_g^-$ above the hypothetical level N=0 of $c^3\Pi_u$; see ^f.
- ^mThe constants refer to N=1 of $r^3\Pi_g^-$; v_{00} is the energy above the hypothetical level N=0 of c(v=0), see ^f.
- ⁿAnticrossings and microwave transitions. The energy difference between $k^3\Pi_u(v=1, N=3)$ and $p^3\Sigma_g^+(v=1, N=5)$ is $+0.2785 \text{ cm}^{-1}$. Fine structure parameters.
- ^o $3A$ of (3); probably a doubly excited state. The possibility (1s δ)(4f π) mentioned by (3) and quoted in MOLSPEC 1 can be ruled out since it does not give rise to an even state.
- $P_{A_0}(\text{ortho}) = -0.00937$, $A_0(\text{para}) = -0.0071_0 \text{ cm}^{-1}$ (123)(133) (154); also hyperfine structure investigated by these authors.
- ^q $w_e y_e = +0.99$ from (15a).
- ^rFrom B_0 and B_1 of Π^- only (1).
- ^sCalculated from the data in (1) and (24). $\Delta G(\frac{1}{2})$ and v_{00} refer to actual N=0 level which is strongly perturbed.
- ^t $3D$ of (4). Probably a doubly excited state: (2p δ)(3d δ).
- ^u $3Y$ of (4). Probably a doubly excited state: (2p δ)(3d π).
- ^vThe T_e values for the upper states of the triplet transitions are based on T_e'' for the lower state (a or c) and have been calculated assuming $Y_{00}' \approx Y_{00}''$.

State	T_e See ^v p.241	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10 ⁻² cm ⁻¹)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
¹ H ₂ (continued)										
j $3\Delta_g$ 3d δ (113533)		2345.2 ₆ ^a	66.5 ₆ ^b	30.08 ₅ ^a	1.69 ₂	1.9 ₀	1.0545	j \leftrightarrow c, ^c R	17633.0 ^p	(1)(24)
i $3\Pi_g$ 3d π (113132)		2253.5 ₅ ^a	67.0 ₅ ^e	29.22 ₁ ^a	1.50 ₆	1.7 ₆	1.0700	i-d, ^f		(132)
								i \rightarrow e, R	5384.81 ^g	(47)
								i \leftrightarrow c, ^c R	17185.8 ^p	(1)(24)
h $3\Sigma_g^+$ 3s σ (112913)		[2268.7 ₃] ^h		[30.6 ₂] ^h			[1.045]	h \rightarrow c,	16990.8 ^d	(2)(24)
g $3\Sigma_g^+$ 3d σ 112854.4		2290.8 ₆	105.4 ₃ ⁱ	j				g \rightarrow e, R	5116.6	(47)
								g \leftrightarrow c, ^c	16917.6 ^d	(1)(2)(24)
d $3\Pi_u$ 3p π 112700.3 ^k		2371.58 ^l	66.27 ^m	30.364 ^{ln}	1.545	[1.91]	1.0496	d ^o \rightarrow a, R	16619.0 ^d	(5)(24)
								Fulcher (α) b.		
e $3\Sigma_u^+$ 3p σ 107774.7		2196.13	65.80 ^q	27.30	1.515		1.107	e \rightarrow a, R	11605.6	(1)(6)
a $3\Sigma_g^+$ 2s σ 95936.1 ^r		2664.83	71.65 ^s	34.216	1.671	[2.16]	0.9887 ₉	a ^t \rightarrow b, ^u		
								(a-X)	95076.4 ^r	
c $3\Pi_u$ 2p π 95838.5 ^v		2466.8 ₉	63.51 ^w	31.07 ^{xy}	1.42 ₅	[1.9 ₅]	1.037 ₆	(c-X)	94881.0 ^z	
b $3\Sigma_u^+$ 2p σ		Unstable; lower state of the continuous spectrum of H ₂ (a \rightarrow b). Pot. function (43).								

¹H₂: ^aThese constants [from (58)] refer to the $3\Pi^-$ and $3\Delta^-$ components and are based on "Approximation 2" of (53) for the evaluation of the l -uncoupling. The observed levels are given by (24).

^b $\omega_e v_e = +0.74_5$.

^cObserved in absorption in flash discharges (60).

^dSee ^f p. 241.

^e $\omega_e v_e = -1.27_2$. Ab initio calculations (41)(45) give a pronounced potential maximum near 2.5 Å for this state.

^fAnticrossings and microwave transitions; i $3\Pi_g$ ($v=3$, $N=2$) is 1.9244 cm^{-1} above d $3\Pi_g$ ($v=3$, $N=1$).

^gRefers to $\Pi^-(N=1)$. $\Pi^+(N=1)$ is at 5471.70 cm^{-1} above e $3\Sigma_u^+$ ($v=0$, $N=0$). The rotational levels are very irregular, only partly on account of l -uncoupling.

^hFrom (24). (2) give $\omega_e = 2395.2$, $\omega_e x_e = 64.2$, $B_0 = 30.0$. According to (24) the $v=0$ levels may be spurious. If so, only $v=1$ remains with $B_1 = 28.7_2$.

ⁱ $\omega_e v_e = +2.40_3$; calculated from the $N=0$ levels of (24).

$^1\text{H}_2$ (continued):

^jSee ^e p. 241.

^kThe fine structure in the $N=1$ levels of both ortho- and para- H_2 has been observed in microwave-optical double resonance by (127) who give $A_e = 0.0281$ as well as spin-spin coupling constants. For para- H_2 , $v=0$, $N=1$ the three component levels $J=1, 2$, and 0 are at -0.01241 , -0.00695 , and $+0.07197 \text{ cm}^{-1}$, resp.. For ortho- H_2 the hyperfine structure has also been studied.

^lConstants refer to $^3\Pi^-$. $^3\Pi^+$ is strongly perturbed, i.e. the Λ -type doubling is fairly large and irregular (7).

^m $w_{ey_e} = + 0.88$.

ⁿBreaking-off of P and R branches ($^3\Pi^+$) above $v'=3$ on account of predissociation. Breaking-off of Q branches ($^3\Pi^-$) for $v'=7, 8$ above $N=1$ on account of preionization (9).

^oLifetime 63 ns (81); see, however, (118) who give 31 ns.

^pLower component of $N'=1$ ($i^3\Pi$) or 2 ($j^3\Delta$) relative to the (non-existent) $N''=0$ level of $c^3\Pi$.

^q $w_{ey_e} = - 0.433$.

^rThe T_0 (v_{00}) value is derived from singlet-triplet anti-crossings in a magnetic field (134)(140) and corresponds to $v=0$, $N=0$. It agrees fairly well with 95073.2 obtained from the energy of a $^3\Sigma_u^+(v=0, N=0)$ below the ionization limit, $29344 \pm 2 \text{ cm}^{-1}$ (9), combined with the new value of I.P. (H_2). (24) gives $T_0 = 95226$ without explanation; the most recent theoretical value is 95077.3 (150). The T_e value in the table takes account of Y_{00} in both upper ($Y'_{00} = 4.92$) and lower state.

^s $w_{ey_e} = + 0.92$. Precise ab initio potential function (incl. diagonal corrections) and predicted vibrational

levels in (67). Except for a constant shift, the latter agree well with the observed levels (24).

^tLifetime $\tau(v=0,1) = 10.4_5 \text{ ns}$ (111)(149).

^uReproduction in MOLSPEC 1, Fig. 12.

^v $A = - 0.1249 \text{ cm}^{-1}$ (135)(138). T_e takes account of Y_{00} in both upper ($Y'_{00} = 4.18$) and lower state.

^w $w_{ey_e} = + 0.552$.

^xThe Λ -type doubling is quite small ($\sim 0.5 \text{ cm}^{-1}$ for $N=6$); the constants refer to the average. The triplet splitting in $N=2$ of para- H_2 has been fully resolved in molecular beam experiments of (28) yielding $\Delta v(J=2-1) = 0.16438$, $\Delta v(J=2-3) = 0.19674 \text{ cm}^{-1}$ with $J=2$ at the top. The hyperfine structure in $N=1, J=2$ of ortho- H_2 is $\Delta v(F=3-2) = 0.0236$, $\Delta v(F=2-1) = 0.0154 \text{ cm}^{-1}$ as quoted by (32). (18) give spin splittings for $N = 1, 2, 3, 4, 5$ without resolving $J=N+1$ from $J=N-1$.

^yThe levels of $c^3\Pi_u^+$ are strongly predissociated by the $b^3\Sigma_u^+$ state (60); the levels of $c^3\Pi_u^-$ are either very weakly affected by a forbidden predissociation to $b^3\Sigma_u^+$ (33) (36) or decay radiatively (by magnetic dipole radiation) to the $b^3\Sigma_u^+$ state as suggested by the lifetime measurements of (117), $\tau(v=0) = 1.02 \text{ ms}$ independent of spin component and isotope. (139) observed quenching of $c^3\Pi_u^-$ in an electric field. The Stark effect is large ($\sim 10^4$ times greater than for the ground state) and has been studied experimentally by (160) and compared with the theoretical values of (145).

^zThis number, obtained from $v_{00}(a-X) + v_{00}(e-a) + v_{00}(g-e) - v_{00}(g-c)$, is 87 cm^{-1} higher than given in MOLSPEC 1, a change made necessary by the work of (47). See also ^r.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-2} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^1\text{H}_2$ (continued)										
Several excited states above the ionization limit, established by electron impact studies and leading to two excited atoms or $\text{H} + \text{H}^+$.										(164)(165)
Continuous absorption above $\sim 130000 \text{ cm}^{-1} \text{ \AA}$.										(38)(49)
$v'=0$ Rydberg series of rotational levels observed in low temperature absorption from $X^1\Sigma_g^+$, $v''=0$, $J''=0$ and 1 and converging to										
$N=2$ of H_2^+ :		$\left\{ \begin{array}{l} J=1 \text{ levels of } \text{np}\pi^1\Pi_u^+ (n = 6, \dots, 32, \text{ joining on to C, D, D', D'')^b; \\ v = 124591.5^c - R/(n+0.082)^2. \text{ Similar series with } v' = 1, \dots, 6^d. \end{array} \right\}$						$R(0)$ lines (para- H_2)	(85)(98) (114)*	
$N=1$ of H_2^+ :		$\left\{ \begin{array}{l} J=1 \text{ levels of } \text{np}\pi^1\Pi_u^- (n = 6, \dots, 43, \text{ joining on to C, D, D', D'')^e; \\ v = 124476.0^c - R/(n+0.082)^2. \text{ Similar series with } v' = 1, \dots, 5. \end{array} \right\}$						$Q(1)$ lines (ortho- H_2)	(85)(98) (114)*	
$N=0$ of H_2^+ :		$\left\{ \begin{array}{l} J=0 \text{ levels of } \text{np}\sigma^1\Sigma_u^+ (n = 5, \dots, 19, \text{ joining on to B, B', B'')^e; \\ v = 124476.0^c - R/(n-0.203)^2. \text{ Similar series with } v' = 1, 2, 3. \end{array} \right\}$						$P(1)$ lines (ortho- H_2)	(98)(114)*	
$N=0$ of H_2^+ :		$\left\{ \begin{array}{l} J=1 \text{ levels of } \text{np}\sigma^1\Sigma_u^+ (n = 5, \dots, 40, \text{ joining on to B, B', B'')^b; \\ v = 124417.2^c - R/(n-0.203)^2. \text{ Similar series with } v' = 1, \dots, 6^d. \end{array} \right\}$						$R(0)$ lines (para- H_2)	(85)(98) (114)*	
$\bar{B}^1\Sigma_u^+$		State causing ion-pair formation after excitation of higher Rydberg states; also responsible for perturbations in $B^1\Sigma_u^+$. Correlates at small r with $B''^1\Sigma_u^+$, forming a double-minimum state								(129)(155) (163).
$D''^1\Pi_u$ 5p π 121211.0 ^f		2319.92 ^f	63.041	30.76 ^{gh}	1.45 ^g	(3)	1.043	$D'' \leftarrow X$, R	120176.0 ^f	(46)(73)
$D'^1\Pi_u$ 4p π 118865.3 ^f		2329.97 ^f	63.140	29.8 ^{ih}	1.11 ⁱ	[2.5] ⁱ	1.058	$D' \leftarrow X$, R	117835.2 ^f	(40)(46)(73)
$S^j 1\Delta_g$ 4d δ [(119893)]		Only $v=0$ observed.		[(28.8)] ^k			[(1.07 ₈)]	$S \rightarrow B$, V	(27510) ^l	(1)(24)
$O^m 1\Sigma_g^+$ 4s σ [(119870)]		Only $v=0$ observed.		[(32)]			[(1.0 ₂)]	$O \rightarrow B$, V	(27487) ⁿ	(1)
$R^o 1\Pi_g$ 4d π (118688)		[2142] ^p		[(30)] ^k			[(1.0 ₆)]	$(R \rightarrow C)$ $R \rightarrow B$, V	(18488) (27376) ^q	(1)(24)
$P^r 1\Sigma_g^+$ 4d σ [119531]		Only $v=0$ observed.		[(30)] ^k			[(1.0 ₆)]	$(P \rightarrow C)$ $P \rightarrow B$, V	18260 27148 ^s	(1)(24)
$T^t 1\Sigma_g^+$ [119512.6]		Only $v=0$ observed.		[(25.4)]			[(1.14 ₈)]	$T \rightarrow B$, V	27130.1	(1)(24)

- ¹H₂: ^aTheoretical and experimental values for the ionization probability into the various vibrational levels of H₂⁺ are given by (50)(71)(75)(147) and (68)(76), resp.. The ionization cross section near the ionization limit has been studied at high resolution by (62)(63). See also (168).
- ^bFor high n there is strong *l*-uncoupling and the two series of ¹Σ_u⁺ and ¹Π_u⁺ levels of para-H₂ should be called np0 and np2, resp., corresponding to the fact that the first converges to N=0, the second to N=2 of H₂⁺. There are strong systematic perturbations between the J=1 levels of these two series (because of *l*-uncoupling) so that the formulae as given do not represent the series very well. An accurate representation can be obtained by Fano's quantum defect theory; see (114). Levels of npπ, ¹Π_u⁺ above N=0 of H₂⁺ are preionized resulting in asymmetrically broadened absorption lines with apparent emission wings.
- ^cLimits of Rydberg series above v''=0, J''=0.
- ^d(155) have observed Rydberg levels with v = 9,10,11 in the study of ion-pair formation.
- ^eThese two series of ortho levels are essentially unperturbed.
- ^fAverage of Π⁺ and Π⁻. v₀₀ referred to {N'=0}.
- ^gRefers to Π⁻; Π⁺ is perturbed, B₀(Π⁺) = 30.178, B₁(Π⁺) = 31.370.

^hRKR potential function in (72).

ⁱRefers to Π⁻; γ_e = - 0.53. Π⁺ is perturbed, B₀(Π⁺) = 31.095, B₁(Π⁺) = 29.165.

^j_{4F} of (24), ⁴₁χ of (1).

^kThe states P, R, S form a d complex with strong uncoupling. As a result the constants given have only limited meaning.

^lThe two J=2 levels are observed at 27631.3 and 27732.9 cm⁻¹ above J=0, v=0 of B ¹Σ_u⁺ (24). The v₀₀ value given is an extrapolated average for J=0 and, because of the uncoupling, is rather uncertain.

^m₄¹0 of (1), not given by (24).

ⁿFrom R(0) and P(1) according to the data of (1).

^o₄¹B of (1), ⁴E of (24).

^pRefers to ¹Π⁻.

^qThe two J=1 levels are observed at 27385.8 and 27487.1 cm⁻¹ above J=0, v=0 of B ¹Σ_u⁺ (24). The v₀₀ value given is an extrapolated average for J=0 and, because of the uncoupling, is rather uncertain.

^r₄¹C of (1), ⁴D of (24).

^sThe J=1 level is observed at 27207.62 cm⁻¹ above J=0, v=0 of B ¹Σ_u⁺. The value given for J=0 is extrapolated and, because of the uncoupling, is rather uncertain.

^t₄¹K of (1), doubly excited state.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
¹ H ₂ (continued)										
B ^u ¹ Σ_u^+ 4p σ	117984.5	2197.50	68.136	26.68 ^{ab}	1.19 ^a	[3.4]	1.119 ₈	B ^u ← X, R	116886.9 ^c	(40)(46)(73) (106)*
N ¹ Σ_g^+ d	(116287)	[1983.3]		[(18.4)]			[(1.35)]	N→B, R	24896.4	(1)(24)
U (¹ Σ_g^+) d	[116707.7]	only v=0.		[(18.8)]			[(1.33)]	U→B, ^e R	24325.1	(1)(24)
M ¹ Σ_g^+ d	(114485)	[2176.0]		[(13)]			[(1.6 ₀)]	M→B, R	23190.0 ^f	(1)(24)
L ¹ Σ_g^+ d	(114520)	[(1835)]		[(9.7)]			[(1.8 ₆)]	L→B, R	23054.8 ^f	(1)(24)
H ^g ¹ Σ_g^+ 3s σ	113899	2538	124	[(29.5)]			[(1.06 ₅)]	H→C, R H→B, V	13866.6 ^h 22754.1 ^h	(1)(24)
D ¹ Π_u 3p π	113888.7	2359.91	68.81 ₆ ⁱ	30.29 ₆ ^{jk}	1.42 ^j	2.01 ^l	1.0508	D→E, R D↔X, ^m R	13709.7 ⁿ 112872.3 ⁿ	(11)(24) (40)* (46) (73)(106)*
J ¹ Δ_g 3d δ	(113550)	2341.1 ₅ ^o	63.2 ₃ ^o	30.08 ₁ ^o	1.71 ₈ ^o	1.8 ₉ ^o	1.0546	J→C, R J→B, ^q V	13435.6 ^p 22322.5 ^p	(1)(24)
I ^r ¹ Π_g 3d π	(113142)	2259.1 ₅ ^o	78.4 ₁ ^{or}	29.25 ₉ ^{os}	1.58 ₄ ^o	1.8 ₀ ^o	1.0693	I ^s →C, R I→B, V	12982.5 ^t 21869.5 ^t	(1)(10)(24)
G ^u ¹ Σ_g^+ 3d σ	112834	2343.9	55.9 ^v	[(28.4)] ^w			[(1.08 ₅)]	G ^w →C, R G→B, ^x V	12722.2 ^y 21609.2 ^y	(1)(24)
K ^z (¹ Σ_g^+)	(112669)	[2232.59]	30	[10.8]			[1.76]	K→C, R K→B, R	12538.6 21425.4	(1)(24)

¹H₂: ^aRepresenting only B₀ and B₁. The B_v curve has a positive curvature for low v and a strong negative curvature for high v. (46) gives B_v = 27.1₃ - 2.35(v+ $\frac{1}{2}$) + 0.665(v+ $\frac{1}{2}$)² - 0.0729(v+ $\frac{1}{2}$)³.

^bRKR potential function (72). Ab initio pot. function (163).

^cDeperturbed value from (40). The observed value for J=0

[perturbed by B'(v=4)] is 116885.6 according to (40) and 116885.3 according to (46), while in the more recent paper (73) gives 116882.00.

^dAll these states are considered as doubly excited states by (24). They may well form one or two double-minimum states (similar to E, F) together with H ¹ Σ_g^+ .

¹H₂ (continued):

^eThis is the $\lambda 4142.8$ progression of (1) as revised by (24).

^fThese values agree with (24); (1) gives 23057.22 and 23191.66 for L and M, respectively.

^g 3^1_0 of (1).

^hFrom R(0) of the 0-0 band and F(1)-F(0) as given by (1).

The basis for 22751.6 in (1) is not clear.

ⁱ $+1.027_4(v+\frac{1}{2})^3 - 0.0420_2(v+\frac{1}{2})^4$; the vibrational constants (73) refer to the average of Π^+ and Π^- . See also ^k.

^j $\gamma_e = -0.025$; the rotational constants (40) represent only the levels $v=0, 1, 2$ of Π^- . The Π^+ levels are strongly perturbed by the B' state which also causes the predissociation of $1^1\Pi^+$ for $v' \geq 3$; see ^k. (46) gives for the deperturbed values

$$B_v(\Pi^+) = 32.5_1 - 2.00(v+\frac{1}{2}) + 0.071(v+\frac{1}{2})^2 - 0.0040(v+\frac{1}{2})^3,$$

$$B_v(\Pi^-) = 30.8_1 - 1.96(v+\frac{1}{2}) + 0.102(v+\frac{1}{2})^2 - 0.0053(v+\frac{1}{2})^3.$$

^kStrong predissociation for $v' \geq 3$; no bands with $v' \geq 3$ have ever been observed in emission. In absorption strongly broadened lines with apparent emission wings (Beutler-Fano shapes) in $D^1\Pi_u^+ \leftarrow X^1\Sigma_g^+$ (106); line widths of 4 and 11.5 cm⁻¹ for J=1 and 2, resp., have been observed (103) and accounted for by interaction with the continuum of $B^1\Sigma_u^+$ (105) (108)(112). Widths for $D^1\Pi_u^- \leftarrow X^1\Sigma_g^+$ (Q) lines are much smaller. Ly α fluorescence as a result of prediss. (63)(82) (97). Electric field induced component of prediss. (92).

^lFrom (40); (46) gives $D_v(\Pi^+) = 0.033 + 0.0010(v+\frac{1}{2})$, $D_v(\Pi^-) = 0.0283 - 0.0012(v+\frac{1}{2})$.

^mRKR Franck-Condon factors (89). Absorption coefficients of D \leftarrow X bands (38). Oscillator strengths $f_{00} = 0.0061_4$, $f_{20} = 0.010_9$ (142).

ⁿAverage of Π^+ and Π^- extrapolated to J=0. The Λ -type doubling for $v=0$, J=1 is 4.2 cm⁻¹ with Π^+ above Π^- .

^oThese constants (58) refer to Π^- and Δ^- and take into account the effects of ℓ -uncoupling in the d complex according to the formulae of (53). They cannot be used to derive energy levels without the use of these formulae. The observed levels are given in (24).

^pRefers to J=2 of Δ^- at 10.8 cm⁻¹ below J=2 of Δ^+ .

^qThe forbidden $1^1\Delta_g \rightarrow 1^1\Sigma_u^+$ transition occurs because of strong uncoupling in the upper state. Only Q branches are observed in these bands.

^r 3^1_B of (1), $3E$ of (24). (39) and (41) predict a fairly high (0.4 eV) maximum in the potential function of this state.

^sZeeman effect studies (20) yield $g(v=0, J=1) = 0.49_8$, $g(v=0, J=2) = 0.41_2$, etc.; lifetime $\tau(v=0, J=2) = 38$ ns (119), see ^w.

^tReferred to J'=1 of $1^1\Pi^-$; J=1 of $1^1\Pi^+$ is 62.32 cm⁻¹ higher.

^u 3^1_C of (1), $3D$ of (24).

^vNo levels higher than $v=3$ have been observed which suggests that the dissociation limit is $1^2S + 2^2S, ^2P$ at 118377.6 cm⁻¹. The constants represent only $v=0, 1, 2$.

^wThis value (1) does not represent the low rotational levels because of ℓ -uncoupling, e.g. the J=1 level is below J=0. The actual levels are given in (24). Hyperfine structure for $v=1, J=1$; $A = 1.0 \pm 0.17$ MHz (136). Large Zeeman splittings corresponding to the strong ℓ -uncoupling (20), $g(v=0, J=1) = 0.90_1$, $g(v=0, J=2) = 0.57_1$, etc.; see also (113). Lifetimes from Hanle effect observations (119); $\tau(v=0, J=1) = 27$ ns, $\tau(v=0, J=2, 3) = 39$ ns.

^xThe G \rightarrow B system gives rise to the strongest lines in the visible region.

^yReferred to J'=0 which, because of ℓ -uncoupling, has an anomalous position.

^z 3^1_K of (1), probably due to $(2s6)^2$.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^1\text{H}_2$ (continued)										
$\text{Q } (^1\Pi_g)^a$ (113163)	[742]			[(16.3)]			[(1.43)]	Q \rightarrow B, R	21151.1	(4)(24)
$\text{B } ^1\Sigma_u^+ 3p6$ 111642.8 ^b	2039.52	83.406 ^c		26.70 ₅ ^e	2.781 ^d	[1.2] ^f	1.119 ₂	B' \rightarrow E, F	11311.5 ^g	(34)
								B' \leftarrow X, ^h R	110478.2	(40)(44)(46)
$\text{F } ^1\Sigma_g^+ \left\{ \begin{array}{l} 2p6^2 \\ 2s6 \end{array} \right. \begin{array}{l} 100911^j \\ 100082.3^m \end{array}$	[1199] ⁱ			$B_4 = 6.24^k$			$r_4 = 2.31_5^k$	F \rightarrow B, ^l R	$\nu_{40} = 13635.1$	(14)(34)
	2588.9 ^m	130.5 ^m		32.68 ^m	1.818 ^m	[2.28] ^m	1.011 ₈	E \rightarrow B, ^l V	8961.23	(8)(22)(24) (34)
$\text{C } ^1\Pi_u 2p\pi$ 100089.8 ⁿ	2443.77	69.524 ^{op}		31.362 ₉ ^p	1.664 ₇ ^q	2.23 ^r	1.0327 ₉	C ^s \leftrightarrow X, ^t R Werner b.	99120.1 ₇ ⁿ	(12)(37)(44) (129)

¹H₂: ^aFragmentary, possibly (2p6)(2p π).

^bTakes account of Y_{00} in both upper and lower state. $Y'_{00} = 15.3 \text{ cm}^{-1}$ is rather uncertain and depends strongly on the number of levels included. See ^d.

^c $+ 3.533(v+\frac{1}{2})^3 - 0.93750(v+\frac{1}{2})^4$; these are the constants of (40) [except T_e which is taken from (129)], they apply only to $v=0, \dots, 4$. (73) gives a very different set of constants based on seven levels $v=0, \dots, 6$. The ΔG curve (in H₂, HD, and D₂) has a characteristic tail which makes representation of the higher vibrational levels by a conventional formula meaningless (40)(129).

^d $+ 0.540(v+\frac{1}{2})^2 - 0.091_7(v+\frac{1}{2})^3$; these constants (40) represent only the first five (deperturbed) B_v values. If only three levels are used $B_v = 26.371 - 1.9000(v+\frac{1}{2}) - 0.0050(v+\frac{1}{2})^2$ leading to a very different Y_{00} value (3.6) from the one used here (see ^b).

^eRKR potential functions (44)(72). A very slight maximum of the potential function at 2.9 \AA has been predicted by (156) but not confirmed in the calculations of (163); see also (151). The experimental data, while suggesting an anomalous form of the potential function, do not indicate a maximum

^fThe higher D_v values are quite irregular. (129).

^gFrom the 0-1 band of (34); from $T_0(B') - T_0(E)$ one obtains 11313.6₂.

^hRKR Franck-Condon factors (89). Oscillator strengths $f_{10} = 0.0028$, $f_{30} = 0.0048$ (142).

ⁱBecause of strong interaction the two states E [² Σ^+ of (1), 2A of (24)] and F, in zero approximation 1s62s6 and (2p6)², form a single state with two minima as first recognized by (30). The most detailed calculation of the potential function and the energy levels is that of (86) whose numbering and $\Delta G(\frac{1}{2})$ value for the F¹ Σ_g^+ component has been adopted in

¹H₂ (continued):

the table. According to (86) ν_{00} (F-B) would be at 9146.8 cm⁻¹ but $\nu=0,1,2,3$ of F have not been observed. The observed $\nu=4$ level lies just below the potential maximum.

^jFrom the observed ν_{40} and the energy of $\nu=4$ above the (outer) minimum as calculated by (86).

^kVibrational numbering of (86). See ⁱ.

^lFranck-Condon factors (137). Electronic trans. moment (88).

^mThese numbers represent only the lower vibrational levels near the inner minimum. Owing to the interaction of E and F (see ⁱ) higher $\Delta G(\nu+\frac{1}{2})$, B_ν , D_ν values are irregular.

ⁿThe T_e values for B and C include the effects of Y_{00} on the zero point energies in both upper and lower states; $Y'_{00}(B) = 8.7$, $Y'_{00}(C) = 5.0$ cm⁻¹. On the other hand, the T_e value of C ¹ Π_u and ν_{00} (C-X) exclude the term $-BA^2$ in the energy formula, a term that is usually included to form part of the effective potential energy. With this inclusion and disregarding Y_{00} (44) gives $T_e = 100063.42$ and $\nu_{00} = 99090.35$ on the basis of older data for $\nu=0\dots4$ and his own precise data for $\nu=5\dots13$.

^o $+0.7312(\nu+\frac{1}{2})^3 - 0.0415(\nu+\frac{1}{2})^4$. These constants refer to the (unperturbed) Π^- component and are based on an 8-level fit to the data of (129) [$\nu=0-4$] and (37) [$\nu=5-7$]. Somewhat different constants are given by (44). Note, that the T_e values in (24) are too low by 8.4 cm⁻¹ (44). The constants of (73) are affected by not recognizing this error.

^pTheoretical work (13)(29)(43)(52)(61) has predicted, and the analysis of the spectrum (40)(129) has confirmed, that

the potential curve of C ¹ Π_u has a van der Waals maximum of ~ 105 cm⁻¹ above the asymptote near $r=4.8$ Å. Ab initio potential function (without diagonal corrections) and predicted vibrational levels (67). RKR potential functions (44) (72); see, however, (124).

^q $+0.0296(\nu+\frac{1}{2})^2 - 0.00296(\nu+\frac{1}{2})^3$. These constants refer to the Π^- component (Π^+ is strongly perturbed by B ¹ Σ_u^+) and are from an 8-level least-squares fit of the data of (129) [$\nu=0-4$] and (37) [$\nu=5-7$]. Somewhat discordant B_ν values for both Π^- and Π^+ (the latter after deperturbation) are given by (37)(46)(129). The Λ -type doubling for $\nu=0$, $J=1$ is 1.17 cm⁻¹; for other ν , J as well as theoretical values see (124)(131).

^r $\beta_e = -0.00074$.

^sLifetime $\tau(\nu=0,1,2,3) = 0.6$ ns (66).

^tRKR Franck-Condon factors calculated by (51)(89) and "measured" by (83)(128)(130) who have also determined the dependence of the transition moment on r . Ab initio calculation of the latter by (88). Theoretical transition probabilities and f values (88)(90)(91)(93), experimental values (66) (130)(142): $f_{10} = 0.059$, $f_{20} = 0.060$, $f_{30} = 0.044$, ... Calculated transitions to the continuum of X ¹ Σ_g^+ (120). Selective enhancements of $\nu=0$ and 2 of C ¹ Π_u in Ar-H₂ mixtures have been studied by (55); similar enhancements have also been observed in Kr-H₂ mixtures. For stimulated emission in the Q(1) and P(3) lines of the 1-4, 2-5, 2-6, 3-7 Werner bands see (116)(121).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^1\text{H}_2$ (continued)										
B $1\Sigma_u^+$ 2p6	91700.0 ^a	1358.09	20.888 ^b	20.015 ₄ ^c	1.1845 ^d	1.625 ^e	1.2928 ₂	$B^f \leftrightarrow X, ^{gh}$ Lyman b.	R 90203.3 ₅	(25)(77)(129)
X $1\Sigma_g^+$ 1s6 ²	0	4401.21 ₃	121.33 ₆ ⁱ	60.853 ₀ ^k	3.062 ₂ ^j	4.71 ^l	0.74144	Quadrupole ^m and field-induced sp.. ⁿ		(15)(48) (26)(56)(74)
								Raman sp.. ^o		(23)(56)
								Rotational ^p and nuclear rf magn. reson.		(17a)(21) (17)(19)

$^1\text{H}_2$: ^aSee ⁿ p. 249.

^b $+ 0.7196(v+\frac{1}{2})^3 - 0.0598(v+\frac{1}{2})^4 + 0.00216(v+\frac{1}{2})^5$, $Y_{00} = 8.7$; from a least squares fit (129) to the first eight levels as given by (25). (77) gives slightly different constants based on the first five levels only. (73) and (37) have observed levels up to $v=35$ and 37, resp., very close to the dissociation limit at 118377.6 cm^{-1} (95). The dissociation energy of the B $1\Sigma_u^+$ state is 28174.2 cm^{-1} .

^cRKR potential functions (31)(44)(72)(89); see also (126). Precise ab initio potential function (incl. diagonal corrections) and predicted vibrational levels (67)(152).

^d $+ 0.1214(v+\frac{1}{2})^2 - 0.0117(v+\frac{1}{2})^3 + 0.0004_6(v+\frac{1}{2})^4$, from a least squares fit (129) to the first eight levels. (77) gives slightly different constants based on the first five levels only. For $v \geq 8$ there are strong rotational perturbations caused by interaction with C $1\Pi_u$. Only after deper-

turbation can meaningful B_v values for these levels be obtained [see (129)]. For a theoretical discussion of the intensities in the perturbed region see (131).

^e $- 2.16_5 \times 10^{-3}(v+\frac{1}{2}) + 2.28_9 \times 10^{-4}(v+\frac{1}{2})^2 - 1.18_5 \times 10^{-5}(v+\frac{1}{2})^3$.

For individual B_v and D_v values see (25)(37)(129).

^fLifetime $\tau(v=3\dots7) = 0.8 \text{ ns}$ (66); $\tau(v=8\dots11) = 1.0 \text{ ns}$ (111).

^gFranck-Condon factors from RKR potentials (51)(89); from ab initio potential functions (64)(90)(91), including theoretical oscillator strengths; see also (167). J dependence of Franck-Condon factors and transition probabilities (87)(88)(102). Experimental Franck-Condon factors and oscillator strengths (57)(65)(69)(83)(130)(142)(157); $\sum f_{v,0} = 0.29$. Variation of transition moment with r (69)(83)(157) and, ab initio, (64)(88). Selective enhancements of $v=3$ and 10 of B $1\Sigma_u^+$ in an Ar- H_2 mixture, first observed by Lyman,

$^1\text{H}_2$ (continued):

have recently been studied by (55); similar enhancements were also observed in Kr- H_2 mixtures. Stimulated emission in the P branches of the 3-10, 4-11, 5-12, 6-13, 7-13 Lyman bands (96)(99).

^hA continuous spectrum corresponding to transitions to the continuum of $X^1\Sigma_g^+$ has been observed (94) and the intensity distribution found to be in agreement with calculations. (93)(120) have calculated transition probabilities and the fractions that go to the continuum for $v'=0\dots 36$. (80) calculated the continuous spectrum corresponding to absorption from the ground state to the continuum of $B^1\Sigma_u^+$. ⁱ $+0.812_9(v+\frac{1}{2})^3$; these constants (56) represent only the levels $v=0,1,2,3$. (25) has less accurate constants representing higher $G(v)$ values. The "true" ω_e (including Dunham corrections) is 4403.2 (48). The zero-point energy ($Y_{00} = 8.9_3$ included) is 2179.2_7 cm^{-1} (27).

^j $+0.057_7(v+\frac{1}{2})^2 - 0.005_1(v+\frac{1}{2})^3$; these constants (56) represent only $B_{0\dots 3}$ which are the best known B_v values. (74) from the field-induced spectrum give a very slightly different B_0 (59.334_3 versus 59.336_2); see also (104). The formula

$B_v = 60.863_5 - 3.0763_8(v+\frac{1}{2}) + 0.0601_7(v+\frac{1}{2})^2 - 0.0048_1(v+\frac{1}{2})^3$ of (25) holds up to $v=8$. Higher B_v values (25) require higher and higher terms in the formula. All the constants given are $Y_{01\dots Y_{31}}$ values; (48) have introduced Dunham

corrections and give the "true" $B_e = 60.867_9$. According to (16) the hyperfine levels $F=1$ and 2 for $J=1, v=0$ are 1.823×10^{-5} and $2.005 \times 10^{-5} \text{ cm}^{-1}$ below the $F=0$ component.

^kRKR potential functions (31)(35)(42), see also (100); ab initio potential functions (141)(153). Rotational and vibrational levels calculated from the latter are given in (153); see also (59)(70). (59) include some of the quasi-bound levels above the dissociation limit [see also (78)]; for their experimental observation see (25)(162). Recent comparisons between ab initio calculated and observed energy levels (115)(144)(158)(159).

^l $-0.0027_4(v+\frac{1}{2}) + 0.0004_0(v+\frac{1}{2})^2$; $H_v = [4.9 - 0.5(v+\frac{1}{2})] \times 10^{-5}$; from (48), see also (56).

^m(48) give absolute intensity measurements of the quadrupole rotation-vibration spectrum (1-0, 2-0, 3-0) as well as corrections for pressure shifts; see also (125)(143)(169). Dependence of quadrupole moment on r (43). Predicted intensities in the rotation-vibration spectrum (84), in the rotation spectrum (110). Predicted lifetimes of rotation-vibration levels (166), e.g. $\tau(v=1, J=1) = 1.17 \times 10^6 \text{ s}$.

ⁿThe rotation and rotation-vibration spectrum has been observed in pressure-induced absorption, see the review by (122).

^oRaman cross sections (148).

^pRotational g factor $g_J = 0.88291$.

$^1\text{H}_2$ (continued):

- (1) Richardson, "Molecular Hydrogen and Its Spectrum", Yale University Press (1934).
- (2) Richardson, Rymer, PRS A 147, 24 (1934).
- (3) Richardson, Rymer, PRS A 147, 251 (1934).
- (4) Richardson, Rymer, PRS A 147, 272 (1934).
- (5) Dieke, Blue, PR 47, 261 (1935).
- (6) Dieke, PR 48, 606 (1935).
- (7) Dieke, PR 48, 610 (1935).
- (8) Dieke, PR 50, 797 (1936).
- (9) Beutler, Jünger, ZP 101, 285 (1936).
- (10) Dieke, Lewis, PR 52, 100 (1937).
- (11) Richardson, PRS A 160, 487 (1937); 164, 316 (1938).
- (12) Dieke, PR 54, 439 (1938).
- (13) King, Van Vleck, PR 55, 1165 (1939).
- (14) Dieke, PR 76, 50 (1949).
- (15) Herzberg, CJR A 28, 144 (1950).
- (15a) Cunningham, Dieke, Report No. NYO-692, Johns Hopkins Univ., Dept. of Physics (1950).
- (16) Ramsey, PR 85, 60 (1952).
- (17) Kolsky, Phipps, Ramsey, Silsbee, PR 87, 395 (1952).
- (17a) Harrick, Ramsey, PR 88, 228 (1952).
- (18) Foster, Richardson, PRS A 217, 433 (1953).
- (19) Harrick, Barnes, Bray, Ramsey, PR 90, 260 (1953).
- (20) Dieke, Cunningham, Byrne, PR 92, 81 (1953).
- (21) Barnes, Bray, Ramsey, PR 94, 893 (1954).
- (22) Porto, Dieke, JOSA 45, 447 (1955).
- (23) Stoicheff, CJP 35, 730 (1957).
- (24) Dieke, JMS 2, 494 (1958).
- (25) Herzberg, Howe, CJP 37, 636 (1959).
- (26) Terhune, Peters, JMS 3, 138 (1959).
- (27) Herzberg, Monfils, JMS 5, 482 (1960).
- (28) Lichten, PR 120, 848 (1960); 126, 1020 (1962).
- (29) Mulliken, PR 120, 1674 (1960).
- (30) Davidson, JCP 35, 1189 (1961).
- (31) Tobias, Vanderslice, JCP 35, 1852 (1961).
- (32) Frey, Mizushima, PR 128, 2683 (1962).
- (33) Lichten, BAPS 7, 43 (1962).
- (34) Porto, Jannuzzi, JMS 11, 379 (1963).
- (35) Weissman, Vanderslice, Battino, JCP 32, 2226 (1963).
- (36) Chiu, JCP 40, 2276 (1964).
- (37) Namioka, JCP 40, 3154 (1964).
- (38) Cook, Metzger, JOSA 54, 968 (1964).
- (39) Mulliken, PR A 136, 962 (1964).
- (40) Namioka, JCP 41, 2141 (1964).
- (41) Browne, PR A 138, 9 (1965).
- (42) Ginter, Battino, JCP 42, 3222 (1965).
- (43) Kolos, Wolniewicz, JCP 43, 2429 (1965).
- (44) Namioka, JCP 43, 1636 (1965).
- (45) Wright, Davidson, JCP 43, 840 (1965).
- (46) Monfils, JMS 15, 265 (1965).
- (47) Gloersen, Dieke, JMS 16, 191 (1965).
- (48) Fink, Wiggins, Rank, JMS 18, 384 (1965).
- (49) Samson, Cairns, JOSA 55, 1035 (1965).
- (50) Dunn, JCP 44, 2592 (1966).
- (51) Halmann, Laulicht, JCP 44, 2398 (1966); 46, 2684 (1967).
- (52) Rothenberg, Davidson, JCP 44, 730 (1966).
- (53) Ginter, JCP 45, 248 (1966).
- (54) Hunter, JCP 45, 3022 (1966).
- (55) Takezawa, Innes, Tanaka, JCP 45, 2000 (1966).
- (56) Foltz, Rank, Wiggins, JMS 21, 203 (1966).
- (57) Geiger, Topschowsky, ZN 21 a, 626 (1966).
- (58) Ginter, JCP 46, 3687 (1967).

$^1\text{H}_2$ (continued):

- (59) Waech, Bernstein, JCP 46, 4905 (1967).
(60) Herzberg, SL 16, 14 (1967).
(61) Kolos, IJQC 1, 169 (1967).
(62) Chupka, Berkowitz, JCP 48, 5726 (1968); 51, 4244 (1969).
(63) Comes, Wellern, ZN 23 a, 881 (1968).
(64) Dalgarno, Allison, ApJ 154, L95 (1968).
(65) Haddad, Lokan, Farmer, Carver, JQSRT 8, 1193 (1968).
(66) Hesser, JCP 48, 2518 (1968).
(67) Kolos, Wolniewicz, JCP 48, 3672 (1968).
(68) Villarejo, JCP 48, 4014 (1968).
(69) Hesser, Brooks, Lawrence, JCP 49, 5388 (1968).
(70) Kolos, Wolniewicz, JCP 49, 404 (1968).
(71) Villarejo, JCP 49, 2523 (1968).
(72) Monfils, BCSARB (5) 54, 44 (1968).
(73) Monfils, JMS 25, 513 (1968).
(74) Brannon, Church, Peters, JMS 27, 44 (1968).
(75) Nicholls, JP B 1, 1192 (1968).
(76) Turner, PRS A 307, 15 (1968).
(77) Wilkinson, CJP 46, 1225 (1968).
(78) Allison, CPL 3, 371 (1969).
(79) Jeziorski, Kolos, CPL 3, 677 (1969).
(80) Allison, Dalgarno, AD 1, 91 (1969).
(81) Cahill, JOSA 59, 875 (1969).
(82) Comes, Wenning, ZN 24 a, 587 (1969).
(83) Geiger, Schmoranz, JMS 32, 39 (1969).
(84) James, JMS 32, 512 (1969).
(85) Herzberg, PRL 23, 1081 (1969).
(86) Kolos, Wolniewicz, JCP 50, 3228 (1969).
(87) Villarejo, Stockbauer, Inghram, JCP 50, 1754 (1969).
(88) Wolniewicz, JCP 51, 5002 (1969).
(89) Spindler, JQSRT 2, 597, 627, 1041 (1969).
(90) Allison, Dalgarno, AD 1, 289 (1970).
(91) Allison, Dalgarno, MP 19, 567 (1970).
(92) Comes, Wenning, ZN 25 a, 406 (1970).
(93) Dalgarno, Stephens, ApJ 160, L107 (1970).
(94) Dalgarno, Herzberg, Stephens, ApJ 162, L49 (1970).
(95) Herzberg, JMS 33, 147 (1970).
(96) Hodgson, PRL 25, 494 (1970).
(97) Mentall, Gentieu, JCP 52, 5641 (1970).
(98) Takezawa, JCP 52, 2575, 5793 (1970).
(99) Waynant, Shipman, Elton, Ali, APL 17, 383 (1970).
(100) Zhirnov, Vasilevskii, OS(Engl. Transl.) 29, 352 (1970).
(101) Stwalley, CPL 6, 241 (1970).
(102) Becker, Fink, ZN 26 a, 319 (1971).
(103) Comes, Schumpe, ZN 26 a, 538 (1971).
(104) Buijs, Gush, CJP 49, 2366 (1971).
(105) Fiquet-Fayard, Gallais, MP 20, 527 (1971).
(106) Herzberg, in "Topics in Modern Physics" (Condon Vol.),
p. 191. Colorado Associated University Press (1971).
(107) Sharp, AD 2, 119 (1971).
(108) Julienne, CPL 8, 27 (1971).
(109) Crosswhite, "The Hydrogen Molecule Wavelength Tables of
Gerhard Heinrich Dieke". Wiley-Interscience (1972).
(110) Dalgarno, Wright, ApJ 174, L49 (1972).
(111) Smith, Chevalier, ApJ 177, 835 (1972).
(112) Fiquet-Fayard, Gallais, CPL 16, 18 (1972).
(113) Freund, Miller, JCP 56, 2211 (1972).
(114) Herzberg, Jungen, JMS 41, 425 (1972).
(115) Bunker, JMS 42, 478 (1972).
(116) Hodgson, Dreyfus, PRL 28, 536 (1972); PR A 2, 2635
(1974).
(117) Johnson, PR A 5, 1026 (1972).
(continued p. 255)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
1H2H		$\mu = 0.67171137$ $D_0^0 = 4.5138_3 \text{ eV}^a$ I.P. = 15.4446_6 eV^b								NOV 1976 A	
k	$3\Pi_u$ 4p π (118384.2)	2030.56	50.36 ^c	22.548	0.951	0.92	1.0550	k \rightarrow a, R	22295.24	(7)	
d	$3\Pi_u$ 3p π (112717.4)	2054.59 ^d	49.74 ^e	22.810 ^{df}	1.020	[1.16]	1.0489	d \rightarrow a, R Fulcher (α) b.	16640.6	(2)	
e	$3\Sigma_u^+$ 3p σ (107776.6)	1905.17	51.70 ^g	20.766	1.010	[0.89]	1.0993	e \rightarrow a, R	11624.6	(1)	
a	$3\Sigma_g^+$ 2s σ (95947.1) ^h	2308.44	53.77 ⁱ	25.685	1.099	[1.28]	0.9885	(a-X)	(95201.5) ^h		
c	$3\Pi_u$ 2p π	No constants of this state have yet been determined. ^j									
b	$3\Sigma_u^+$ 2p σ	Repulsive, lower state of hydrogen continuum.							a \rightarrow b		

¹_H²H: ^a36406.2 cm⁻¹, from (29). From ab initio calculations (21) obtain 36405.5 cm⁻¹, including a very small non-adiabatic correction by (51).

^bFrom the Rydberg series of (36) and corrected for pressure shift, see (34).

^c $w_e y_e = + 0.6968$.

^dRefers to $3\Pi^-$; $3\Pi^+$ is strongly perturbed.

^e $w_e y_e = + 0.58$.

^fThe Λ -type doubling is large and irregular (1). Breaking-off of P and R branches for $v' > 3$ on account of predissociation (2).

^g $w_e y_e = + 0.522$, $w_e z_e = + 0.091$.

^hThe energy of none of the triplet states above X $1\Sigma_g^+(v=0, J=0)$ has yet been experimentally established. The T_e value in the table is the average of those of H₂ and D₂; the electronic isotope shift is fairly large. T_0 is calculated from this T_e value taking account of $Y'_{00} = 3.8_5$. The theoretical $T_e = 95950 \text{ cm}^{-1}$ is based on the observed dissociation limit and D_e from (17).

ⁱ $w_e y_e = + 0.60$.

^jSee footnote ^y on p. 243 (¹H₂).

¹H₂ (continued):

- (118) Marechal, Jost, Lombardi, PR A 5, 732 (1972).
(119) Van der Linde, Dalby, CJP 50, 287 (1972).
(120) Stephens, Dalgarno, JQSRT 12, 569 (1972).
(121) Waynant, PRL 28, 533 (1972).
(122) Welsh, in MTP Review of Science, Phys.Chem. Ser. 1, Vol. 3, p. 33 (1972); PC 30, 84 (1974).
(123) Freund, Miller, Zegarski, CPL 23, 120 (1973).
(124) Julienne, JMS 48, 508 (1973).
(125) Margolis, JMS 48, 409 (1973).
(126) Stwalley, JCP 58, 536 (1973).
(127) Freund, Miller, JCP 58, 2345, 3565; 59, 4093, 5770 (1973).
(128) Schmoranzner, Geiger, JCP 59, 6153 (1973).
(129) Dabrowski, Herzberg, CJP 52, 1110 (1974).
(130) Fabian, Lewis, JQSRT 14, 523 (1974).
(131) Ford, JMS 53, 364 (1974).
(132) Freund, Miller, JCP 60, 4900 (1974).
(133) Miller, Freund, Zegarski, JCP 60, 3195 (1974).
(134) Miller, Freund, JCP 61, 2160 (1974); 63, 256 (1975).
(135) Jette, JCP 61, 816 (1974).
(136) Melieres-Marechal, Lombardi, JCP 61, 2600 (1974).
(137) Lin, JCP 60, 4660 (1974).
(138) Jette, Miller, CPL 29, 547 (1974).
(139) Johnson, PR A 2, 576 (1974).
(140) Jost, Lombardi, PRL 33, 53 (1974).
(141) Kolos, Wolniewicz, CPL 24, 457 (1974).
(142) Lewis, JQSRT 14, 537 (1974).
(143) McKellar, Icarus 22, 212 (1974).
(144) Orlikowski, Wolniewicz, CPL 24, 461 (1974).
(145) English, Albritton, JP B 8, 2123 (1975).
(146) Ford, JMS 56, 251 (1975).
(147) Ford, Docken, Dalgarno, ApJ 195, 819; 200, 788 (1975).
(148) Harney, Randolph, Milanovich, ApJ 200, L179 (1975).
(149) King, Read, Imhof, JP B 8, 665 (1975).
(150) Kolos, CPL 31, 43 (1975).
(151) Wolniewicz, CPL 31, 248 (1975).
(152) Kolos, Wolniewicz, CJP 53, 2189 (1975).
(153) Kolos, Wolniewicz, JMS 54, 303 (1975).
(154) Miller, Freund, JCP 62, 2240 (1975).
(155) Chupka, Dehmer, Jivery, JCP 63, 3929 (1975).
(156) Ford, Browne, Shipsey, DeVries, JCP 63, 362 (1975).
(157) Schmoranzner, JP B 8, 1139 (1975).
(158) Dabrowski, Herzberg, CJP 54, 525 (1976).
(159) Bishop, Shih, JCP 64, 162 (1976).
(160) Kagann, English, PR A 13, 1451 (1976).
(161) Bunker, unpublished.
(162) Herzberg, McKenzie, to be published.
(163) Kolos, JMS 62, 429 (1976).
(164) Crowe, McConkey, PRL 31, 192 (1973).
(165) Misakian, Zorn, PR A 6, 2180 (1972).
(166) Black, Dalgarno, ApJ 203, 132 (1976).
(167) Lin, CJP 53, 310 (1975).
(168) Backx, Wight, Van der Wiel, JP B 9, 315 (1976).
(169) Chackerian, Giver, JMS 58, 339 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^1\text{H}^2\text{H}$ (continued)		Ionization continua joining on to Rydberg series. ^a								
Rydberg series of rotational levels observed in low temperature absorption from $X^1\Sigma_g^+(v=0)$ and converging to										
N=2 ($v=1$) of HD^+ :	{J=1 ($v=1$) levels of $np\pi$ $^1\Pi_u^+$ ($n = 36\dots 46$) ^{bc} ; $v = 126606.4^d - R_{\text{HD}}/(n+0.082)^2$.						R(0) lines	(36)		
N=1 ($v=0$) of HD^+ :	{J=1 ($v=0$) levels of $np\pi$ $^1\Pi_u^-$ ($n = 6\dots 23$, joining on to C, D, D', D''); $v = 124613.3^d - R_{\text{HD}}/(n+0.082)^2$. Similar series with $v' = 1, 2, 3$.						Q(1) lines	(36)		
N=0 ($v=0$) of HD^+ :	{J=1 ($v=0$) levels of $np\sigma$ $^1\Sigma_u^+$ ($n = 5\dots 48$, joining on to B, B', B'') ^c ; $v = 124568.6^d - R_{\text{HD}}/(n-0.203)^2$. Similar series with $v' = 1$.						R(0) lines	(36)		
$\bar{B}^1\Sigma_u^+$	See $^1\text{H}_2$.							(42)(46)		
D'' $^1\Pi_u$ 5p π	121231.2 ^e 121216.3 ^e	2006.17 ^f	45.801 ^f	[22.865] ^g [22.144]	h	[2.1] [1.3]	[1.0477] [1.0646]	D'' \leftarrow X, R	120332.6 ^e 120317.7 ^e	(13)(18)
D' $^1\Pi_u$ 4p π	118879.2 ^f	2014.9 ₁ ^f	47.018 ⁱ	22.3 ₅ ^g	1.25 ^k	[2.2] ^j	1.060	D' \leftarrow X, R	117984.7	(13)(18)
B'' $^1\Sigma_u^+$ 4p σ	117980.4	1896.60	48.924	20.34 ^l	0.398 ^l	[2.5]	1.111	B'' \leftarrow X, R	117026.2	(13)(18)
M $^1\Sigma_g^+$	[115073]	v=0 (?) only.		[10.4]			[1.55]	M \rightarrow B, R	22782.5	(4)
D $^1\Pi_u$ 3p π	113901.7 ^m	2039.13 ^f	48.91 ₇ ⁿ	22.9 ₁ ^{og}	0.97 ^p	(1.2) ^q	1.047	D \leftarrow X, ^r R	113018.8 ₄ ^s	(13)(18)
J $^1\Delta_g$ 3d δ	(113536)	[1832.8] ^t						J \rightarrow B, V	22162.3 ^t	(4)
I $^1\Pi_g$ 3d π	(113110)	1962.14 ^o	58.21 ^u	22.36 ^o	1.21	[0.7]	1.059	I \rightarrow B, V	21786.2 ^v	(4)
G $^1\Sigma_g^+$ 3d σ	(112843)	[1879.9], vibrational perturbations for $v > 0$. ^u						G \rightarrow B, R	21492.4	(4)
K ($^1\Sigma_g^+$)	(112663)	[(1981)], only fragmentary data.						K \rightarrow B, R	(21363.2) ^w	(4)
B' $^1\Sigma_u^+$ 3p σ	111649.7 ^x	1775.2	67.6 ₆ ^{yu}	20.0 ₀ ^{zg}	1.2 ₈ ^z	[0.16] ^z	1.120	B' \leftarrow X, ^r R	110632.5 ₈	(13)(18)(48)

¹H²H: ^aCross sections for photoionization into the various vibrational levels of HD⁺ and the adjoining continuum (dissociative photoionization) calculated by (39)(44), observed by (37). Photoionization near I.P. studied by (12).
^bExcept for n=2...5 (i.e. C...D") only the diffuse (pre-ionized) members above n=35 have been observed. The corresponding v'=0 series has not been found for n>5.
^cThere are strong perturbations between npσ¹Σ_u⁺ and npπ¹Π_u⁺ similar to those in H₂, but in HD they have not yet been studied in detail.
^dThe Rydberg limits are from (36) but corrected for pressure shift; see (34). The quantum defects, given only for the Q(1) series by (36), are taken from the corresponding series in H₂ (34).
^eLarge J=0 splitting (18), Π⁺ above Π⁻.
^fAverage of Π⁺ and Π⁻ which differ for HD much more than for H₂ and D₂.
^gRKR potential functions (19).
^hB₁(Π⁺) = 22.618, B₁(Π⁻) = 22.310.
ⁱw_ev_e = + 0.126₆.
^jThe rotational constants refer to Π⁻; Π⁺ is perturbed (see ^c); B₀(Π⁺) = 22.289, B₁(Π⁺) = 21.901.
^kγ_e = - 0.05.
^lThe rotational constants represent B₀ and B₁ only; strongly non-linear B_v curve.
^mY₀₀ not included. (18) gives 113900.7₅.
ⁿw_ev_e = + 0.2171.
^oRefers to Π⁻.

pγ_e = - 0.028.

^qThe D_v values show considerable scatter. The H_v values (13) are hardly significant.

^rFranck-Condon factors from electron energy loss spectra in (26).

^sAverage of Π⁺ and Π⁻, extrapolated to J=0. The Λ-type doubling for J=1, v=0 is 3.5₂ cm⁻¹ with Π⁺ above Π⁻.

^tReferred to J=2 of ¹Δ⁻.

^uThere are two dissociation limits with adjoining continua at 118665.9 and 118687.4 cm⁻¹ corresponding to H(n=2) + D(n=1) and H(n=1) + D(n=2), respectively (29). It appears (48) that the first limit corresponds to B¹Σ_u⁺, E, F¹Σ_g⁺, and C¹Π_u, while the second corresponds to B'¹Σ_u⁺, G¹Σ_g⁺, and I¹Π_u; see also (32). The C¹Π_u state, unlike H₂ or D₂, apparently does not have a potential maximum.

^vRefers to J=1 of Π⁻; J=1 of Π⁺ lies 28.0 cm⁻¹ higher.

^wRefers to the J=1 level.

^xTakes account of Y₀₀ in the upper as well as in the lower state. For the states B, C, and B' Y'₀₀ = 7.1, 3.7, and 2.0, respectively.

^yw_ev_e = + 3.6₆, w_ez_e = - 0.6₅; five-level fit. All levels up to the last (v=11) have been observed.

^zFive-level fit. The deviations for v>2 are large and irregular because of numerous perturbations. The B_v values of (13) deviate by up to 1 cm⁻¹ from those of (48) used here. The latter are effective, non-deperturbed values. Higher D_v values show considerable irregularities because of local perturbations.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^1\text{H}^2\text{H}$ (continued)										
$F^a \left\{ \begin{array}{l} 1\Sigma^+ \\ 2\Sigma^+ \end{array} \right\} 2p6^2$	100927.5 ^b	(1087.9) ^c	(21.6) ^{cd}	$B_1 = 4.50$			$r_1 = 2.36$	E→B, V	8901.72	(3)(48)
$E^a \left\{ \begin{array}{l} 1\Sigma^+ \\ 2\Sigma^+ \end{array} \right\} 2s6$	100120.4 ^b	2204.4 ^e	81.6 ^e	24.568 ^e	1.288 ^e	[1.23]	1.0107	E,F←X, ^f R	99301.5 ^g	(48)*
C $^1\Pi_u$ 2p π	100092.9 ^h	2119.6 ₅	53.31 ⁱ	23.522 ^j	1.096 ^k	1.4 ₉ ^l	1.0329	C↔X, ^{my} R Werner b.	99252.8 ₆	(13)(18)(48)
B $^1\Sigma_u^+$ 2p σ	91698.3 ^h	1177.16	15.59 ⁿ	15.071 ^j	0.820 ^o	0.882 ^p	1.2904	B↔X, ^{qy} R Lyman b.	90399.8 ₆	(23)* (48)*
X $^1\Sigma_g^+$ 1s6 ²	0	3813.1 ₅	91.65 ^r	45.655 ^s	1.986 ^t	2.60 ₅ ^u	0.74142	Rotation-vibration sp. ^v Pure rotation sp. ^w Raman sp. Field- and collision-induced sp. Rf magn. reson. sp. ^x		(10)(49) (22) (9) (20) (45) (5)(6)

$^1\text{H}^2\text{H}$: ^aThe states E and F may be considered as forming one double-minimum state. The potential maximum is at 104480 cm^{-1} above $X(v=0, J=0)$ (27). See also ⁱ on p. 248 ($^1\text{H}_2$).

^bDerived by extrapolation of differences between observed vibrational levels (48) and those calculated from the double-minimum potential function of (27).

^cFrom the theoretical energy levels assuming an independent (outer) potential minimum (48). The lowest observed level is $v=1$ and the observed intervals are $\Delta G(3/2, 5/2, 7/2) = 1002.6, 956.0, 916.7$, resp.. Higher levels show the effects of interaction with $E \ ^1\Sigma_g^+$. See ^a.

^dSee ^u p. 257.

^eThese constants (3) are from the lowest vibrational levels ($v \leq 2$ of the inner minimum) neglecting the interaction with the F state; see ^a.

^fThis transition, forbidden in H_2 and D_2 , is weakly allowed in HD since the g, u symmetry is no longer rigorous.

^gThe 0-0 band has not been observed in VUV absorption but is obtained by adding $\nu_{00}(E-B)$ (3) to $\nu_{00}(B-X)$. The first observed VUV absorption band is at 100618.50 cm^{-1} and corresponds to the transition to the second lowest level in the outer minimum (1-0).

¹H²H (continued):

^hSee ^xp. 257. Note, that the T_e value for C ¹Π_u and $v_{00}(C-X)$ exclude the term $-BA^2$ of the rotational energy expression.

ⁱ $w_e v_e = + 0.656$, $w_e z_e = - 0.033$; eight-level fit. Only Π⁻ levels have been included in the fit since many of the Π⁺ levels are strongly perturbed by B ¹Σ_u⁺. After deperturbation the Π⁺ levels agree fairly well with corresponding Π⁻ levels. Levels up to $v=15$ have been observed; this level is within 42 cm⁻¹ of the lower of the two dissociation limits, see ^up. 257.

^jRKR potential functions (19).

^k $+ 0.037(v+\frac{1}{2})^2 - 0.0053(v+\frac{1}{2})^3$, eight-level fit of B_v values of Π⁻.

^l $\beta_e = - 0.00077$.

^mSelective enhancement of $v'=0$ of C ¹Π in Ar-H₂ mixtures studied by (15). Franck-Condon factors from electron energy loss spectra (26).

ⁿ $+ 0.427(v+\frac{1}{2})^3 - 0.029(v+\frac{1}{2})^4 + 0.0008(v+\frac{1}{2})^5$, fit of first eight levels; all levels up to $v=43$ have been observed (48).

^o $+ 0.116(v+\frac{1}{2})^2 - 0.0216(v+\frac{1}{2})^3 + 0.0024(v+\frac{1}{2})^4 - 0.00011(v+\frac{1}{2})^5$; eight-level fit, see ⁿ.

^p $\beta_e = - 0.000505$.

^qSelective enhancement of $v'=3$ and 5 of B ¹Σ_u⁺ in Ar-H₂ mixtures studied by (15). Franck-Condon factors from electron energy loss spectra (26), from fluorescence spectra (25); large vibration-rotation interaction effects (25)(28)(30).

^r $+ 0.723(v+\frac{1}{2})^3 - 0.0133(v+\frac{1}{2})^4 + 0.00165(v+\frac{1}{2})^5$; ten-level fit. The zero-point energy ($Y_{00} = 6.51$ included) is 1890.2₆. All levels up to the last, $v=17$, have been observed. This level lies 5.1 cm⁻¹ below the dissociation limit.

^sTheoretical values for all bound and quasibound levels in the ground state of HD are given by (31).

^t $+ 0.0315(v+\frac{1}{2})^2 - 0.00221(v+\frac{1}{2})^3$; ten-level fit (48). Somewhat more accurate B_v values than used by (48) for $v=0...6$ have been derived from the rotation-vibration spectrum by (49).

^u $\beta_e = - 0.00054$; $H_v = 2.2 \times 10^{-5}$ has been assumed.

^vThe transition moments for the 1-0, 2-0, 3-0, 4-0 and 5-0 vibration bands are observed to be 5.0, 1.9, 0.80, 0.42 and 0.21×10^{-5} D, respectively (40)(41)(43)(49); for theoretical discussions see (38)(47)(50). In addition to the electric dipole infrared spectrum one line of the quadrupole component of the fundamental, S(0), has been observed (43).

^wFrom the rotation spectrum (22) have obtained a dipole moment in the lowest vibrational level of 5.8×10^{-4} D, or, after a small correction for rotation (16), 5.5×10^{-4} D; see also (38). Predicted IR emissivities in the pure rotation lines (33).

^xRotational magnetic moment for $J=1$ 0.662 μ_N (6)(8).

^yTheoretical band oscillator strengths, transition probabilities and photodissociation cross sections in (24).

References on page 261.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
H ³ H		$\mu = 0.75540394$ $D_0^0 = (4.5269_4) \text{ eV}^a$ I.P. = $(15.4514_6) \text{ eV}^b$								NOV 1976
k	$3\Pi_u$ 4p π (118384.8)	1915.05	44.67 ^c	20.106	0.8638 ^d	0.86	1.0535	k \rightarrow a, R	22303.7 ₈	(2)
d	$3\Pi_u$ 3p π (112717.9)	1936.93	43.439 ^e	20.219 ^f	0.823 ^f	0.812 ^g	1.0506	d \rightarrow a, R	16648.1 ₀	(1)
e	$3\Sigma_u^+$ 3p σ (107772.7)	1796.42	45.69 ^h	18.3167	0.819 ⁱ	0.744 ^j	1.1037 ₉	e \rightarrow a, R	11631.98	(3)
a	$3\Sigma_g^+$ 2s σ (95950.8) ^k	2177.01	47.84 ^l	22.819	0.9182 ^m	0.97 ⁿ	0.9889 ₂	(a-X)	(95243.5) ^o	
C	$1\Pi_u$ 2p π (100094.7) ^k							(C-X)	(99301.5) ^p	
B	$1\Sigma_u^+$ 2p σ (91698.1) ^k							(B-X)	(90472.2) ^p	
X	$1\Sigma_g^+$ 1s σ^2 0	3597.0 ₅ ^q	81.67 ₈ ^q	40.595	1.6640 ^r		(0.74142)			

$1H^3H$, $a_{36511.9} \text{ cm}^{-1}$, from ab initio potential function (7); non-adiabatic corrections which are certainly less than $+0.35 \text{ cm}^{-1}$ and Lamb shift corrections ($\approx -0.2 \text{ cm}^{-1}$) are not included. No observed value is available yet.

^bFrom theoretical $D_0^0(\text{HT})$ and $D_0^0(\text{HT}^+)$ values and I.P.(H).

^c $w_e v_e = +0.527$.

^d $r_e = +0.0123$.

^e $w_e v_e = +0.459$, $w_e z_e = -0.036$.

^f $r_e = +0.0080$; the rotational constants refer to $3\Pi^-$ since $3\Pi^+$ is perturbed; the Λ -type doubling is somewhat irregular and fairly large.

^g $\beta_e = -0.00008$.

^h $w_e y_e = +0.34$, $w_e z_e = -0.060$.

ⁱ $r_e = -0.0039$.

^j $\beta_e = -0.00041$.

^kFrom the T_e values of H_2 and D_2 assuming that the electro-nic isotope shift is proportional to $(1 - \mu_{H_2}/\mu_{HT})$.

^l $w_e y_e = +0.502$, $w_e z_e = -0.015$.

^m $r_e = +0.0123$.

ⁿ $\beta_e = -0.00038$.

^oFrom T_e assuming $Y_{00}^0 = 0$, but taking account of Y_{00}^0 (see ^q).

^pFrom T_e and the zero-point energy calculated by (6).

^qAll constants calculated by (5) from the potential function of (4) and based on $v=0,1,2,3$ only. Experimental values are not available. $w_e y_e = +0.575$; $Y_{00} = 5.7$. $r + 0.0238(v+\frac{1}{2})^2 - 0.0015(v+\frac{1}{2})^3$. See also ^q.

$^1\text{H}^3\text{H}$ (continued):

- (1) Dieke, Tomkins, PR 76, 283 (1949).
- (2) See ref. (15a) of $^1\text{H}_2$.
- (3) Dieke, Tomkins, PR 82, 796 (1951).

- (4) See ref. (43) of $^1\text{H}_2$.
- (5) Cashion, JCP 45, 1037 (1966).
- (6) See ref. (67) of $^1\text{H}_2$.
- (7) See ref. (70) of $^1\text{H}_2$.

$^1\text{H}^2\text{H}$ (continued):

- (1) See ref. (6)(7) of $^1\text{H}_2$.
- (2) See ref. (5) of $^1\text{H}_2$.
- (3) See ref. (8) of $^1\text{H}_2$.
- (4) See ref. (10) of $^1\text{H}_2$.
- (5) Kellogg, Rabi, Ramsey, Zacharias, PR 57, 677 (1940).
- (6) Ramsey, PR 58, 226 (1940).
- (7) See ref. (15a) of $^1\text{H}_2$.
- (8) Ramsey, "Molecular Beams", p. 239. Clarendon Press, Oxford (1956).
- (9) See ref. (23) of $^1\text{H}_2$.
- (10) Durie, Herzberg, CJP 38, 806 (1960).
- (11) Blinder, JCP 35, 974 (1961).
- (12) Dibeler, Reese, Krauss, JCP 42, 2045 (1965).
- (13) See ref. (46) of $^1\text{H}_2$.
- (14) Kolos, Wolniewicz, JCP 45, 944 (1966).
- (15) Takezawa, Innes, Tanaka, JCP 46, 4555 (1967).
- (16) Karl, CJP 46, 1973 (1968).
- (17) See ref. (67) of $^1\text{H}_2$.
- (18) See ref. (73) of $^1\text{H}_2$.
- (19) See ref. (72) of $^1\text{H}_2$.
- (20) See ref. (74) of $^1\text{H}_2$.
- (21) See ref. (70) of $^1\text{H}_2$.
- (22) Treffler, Gush, PRL 20, 703 (1968); CJP 47, 2115 (1969).
- (23) See ref. (77) of $^1\text{H}_2$.
- (24) See ref. (80)(90)(91) of $^1\text{H}_2$.
- (25) Fink, Akins, Moore, CPL 4, 283 (1969).

- (26) See ref. (83) of $^1\text{H}_2$.
- (27) See ref. (86) of $^1\text{H}_2$.
- (28) Allison, JCP 52, 4909 (1970).
- (29) See ref. (95) of $^1\text{H}_2$.
- (30) See ref. (102) of $^1\text{H}_2$.
- (31) Le Roy, JCP 54, 5433 (1971).
- (32) Thorson, JMS 37, 199 (1971).
- (33) See ref. (110) of $^1\text{H}_2$.
- (34) See ref. (114) of $^1\text{H}_2$.
- (35) See ref. (117) of $^1\text{H}_2$.
- (36) Takezawa, Tanaka, JCP 56, 6125 (1972).
- (37) Berkowitz, Spohr, JESRP 2, 143 (1973).
- (38) Bunker, JMS 46, 119 (1973).
- (39) Itikawa, JESRP 2, 125 (1973).
- (40) McKellar, CJP 51, 389 (1973).
- (41) Bejar, Gush, CJP 52, 1669 (1974).
- (42) See ref. (129) of $^1\text{H}_2$.
- (43) McKellar, CJP 52, 1144 (1974).
- (44) See ref. (147) of $^1\text{H}_2$.
- (45) Prasad, Reddy, JCP 62, 3582 (1975); 65, 83 (1976).
- (46) See ref. (155) of $^1\text{H}_2$.
- (47) Bunker, JMS 61, 319 (1976).
- (48) See ref. (158) of $^1\text{H}_2$.
- (49) McKellar, Goetz, Ramsay, ApJ 207, 663 (1976).
- (50) Wolniewicz, CJP 53, 1207 (1975); 54, 672 (1976).
- (51) Bunker, unpublished.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^2\text{H}_2$										
		$\mu = 1.00705111$	$D_0^0 = 4.55632 \text{ eV}^a$		$\text{I.P.} = 15.46660 \text{ eV}^b$				NOV 1976 A	
u $^3\Pi_u$ 6p π 122365.6	1649.03	35.13 ^c	15.03 ₆	0.587 ^d	0.53	1.055 ₁	u \rightarrow a,	26286.75	(6)	
w ($^3\Pi_g$) 5d π	Fragment						w \rightarrow c,		(6)	
q ($^3\Sigma_g^+$) 5d σ	Fragment						q \rightarrow c,		(6)	
n $^3\Pi_u$ 5p π 120976.9	1652.73	34.25 ^e	15.04 ₀ ^f	0.560 ^g	0.53	1.055 ₀	n \rightarrow a,	24900.14	(6)	
r $^3\Pi_g$ 4d π [(119380)]			hi				r \rightarrow c, R	(22650) ^h	(6)	
p $^3\Sigma_g^+$ 4d σ [119242]			h				p \rightarrow c, R	22509.9 ^h	(6)	
k $^3\Pi_u$ 4p π 118396.7	1658.85	33.88 ^j	15.07 ₅ ^k	0.566 ^l	0.46	1.053 ₈	k \rightarrow a,	22323.06	(6)	
f $^3\Sigma_u^+$ 4p σ 116640	1618	32.8	14.66	0.62		1.069	f \rightarrow a, R	20546.0	(6)	
j $^3\Delta_g$ 3d δ [114194.1]			h				j \rightarrow c, V	17462.3 ^h	(6)	
i $^3\Pi_g$ 3d π (113093)	[1541.9]		hm				i \rightarrow e, R	5320.0 ⁿ	(15)*	
							i \rightarrow c, R	17131.9 ⁿ	(6)	
g $^3\Sigma_g^+$ 3d σ (112856)	[1511.3]		h				g \rightarrow e, R	5067.8	(15)*	
							g \rightarrow c, R	16879.8	(6)	
d $^3\Pi_u$ 3p π 112729.8 ^o	1678.22 ^p	32.94 ^q	15.200 ^p	0.5520	[0.49]	1.0494	d \rightarrow a, R	16666.0	(1)	
e $^3\Sigma_u^+$ 3p σ 107774.0	1556.64	34.51 ^r	13.856	0.451	[0.4]	1.0991	Fulcher b.			
a $^3\Sigma_g^+$ 2s σ 95958.0 ^s	1885.84	35.96 ^s	17.109	0.606	[0.55]	0.9891	e \rightarrow a, R	11649.1	(2)	
							a ^t \rightarrow b,			
c $^3\Pi_u$ 2p π [96731.8]			[15.305] ^v		[0.514] ^v	[1.0458]	(a-X)	95348.1 ₈ ^u	(1)	
b $^3\Sigma_u^+$ 2p σ	Lower state of continuous spectrum of D ₂ (a \rightarrow b).						(c ^w -X)	95185.3 ^x	(6)	

$^2\text{H}_2$: ^a36748.9 cm^{-1} , from the dissociation limit (beginning of continuum) in the B'-X system (34). The same value has been derived by (53) from the last observed levels in the ground state by relations involving the long-range behaviour of the potential function. 36748.2 cm^{-1} from ab initio calculations (52).

^bFrom the Rydberg limits of (54) after correction for pressure shift (41).

^c $w_e y_e = + 0.627$, uncertain.

^d $y_e = + 0.008$, uncertain.

^e $w_e y_e = + 0.627$, uncertain.

^f Λ -type doubling constant $q(v=0) = 0.25 \text{ cm}^{-1}$ (6).

^g $y_e = + 0.035$.

^hStrongly affected by ℓ -uncoupling, no constants given by (6); v_{00} roughly evaluated from their wave number data. See also ^e and ^k p. 241 ($^1\text{H}_2$).

ⁱAnti-crossings of $r \ ^3\Pi_g(v=0, N=2)$ with $G \ ^1\Sigma_g^+(v=4, N=2)$ yielding orbital g factors and hyperfine structure (57).

^j $w_e y_e = + 0.508$, $w_e z_e = + 0.0345$.

^k Λ -type doubling constant $q(v=0) = 0.29 \text{ cm}^{-1}$ (6).

^l $y_e = + 0.008$, uncertain.

^mAnti-crossings between $i \ ^3\Pi_g(v=1, N=1)$ and $I \ ^1\Pi_g(v=1, N=1)$ observed by (56).

ⁿRefers to $\Pi^-(v=0, N=1)$; $\Pi^+(v=0, N=1)$ is at 5348.9 cm^{-1}

above $e \ ^3\Sigma_u^+(v=0, N=0)$. The rotational levels are very irregular.

^oMicrowave optical magnetic resonance induced by electrons (45) gives the following triplet splittings for $v=0, N=1$ of para- D_2 : $\Delta v_{10} = 0.04301$, $\Delta v_{02} = 0.00656$, and of ortho- D_2 : $\Delta v_{02} = 0.08286$, $\Delta v_{21} = 0.00402 \text{ cm}^{-1}$; similar splittings for $v=1\dots 5$. (47) derive $A_e = - 0.02809 \text{ cm}^{-1}$.

^pRefers to the $^3\Pi^-$ component; $^3\Pi^+$ is strongly perturbed. The Λ -type doubling is large and irregular (3); for $v=0, N=1$ it is 0.13 cm^{-1} (47). Breaking-off of P and R branches for $v' > 4$ on account of predissociation (1); see also (45).

^q $w_e y_e = + 0.24$.

^r $w_e y_e = + 0.287$, $w_e z_e = - 0.04$.

^s $w_e y_e = + 0.34$. T_e takes account of Y_{00} in both upper ($Y'_{00} = 2.6_7$) and lower state.

^tLifetime $\tau(v=0, 1) = 12.5 \text{ ns}$ (42).

^uFrom singlet-triplet anti-crossings (56)(57).

^vFrom the assignments of (6) in the g-c, i-c, j-c, ... bands by evaluating combination differences.

^wLifetime $\tau(v=0) = 1.02 \text{ ms}$ (42a), refers to the non-predissociating component $c \ ^3\Pi_u^-$ and corresponds to radiative (magnetic dipole) transitions to $b \ ^3\Sigma_u^+$; see ^y p. 243 ($^1\text{H}_2$).

^xFrom T_0 of a $^3\Sigma_g^+$ and the v_{00} values for the transitions e-a, g-e, and g-c.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^2\text{H}_2$ (continued)		Ionization continua joining on to Rydberg series. ^a								
$v'=0$ Rydberg series of rotational levels observed in low temperature absorption from $X^1\Sigma_g^+(v=0)$ and converging to										
N=2 of D_2^+ :		{J=1 levels of $np\pi \ ^1\Pi_u^+$ ($n = 6...9$, joining on to C, D, D', D'') ^b ; $v = 124833 - R_{D_2}/(n+0.082)^2$.						R(0) lines (ortho- D_2)	(54)	
N=1 of D_2^+ :		{J=1 levels of $np\pi \ ^1\Pi_u^-$ ($n = 6...24$, joining on to C, D, D', D'') ^c ; $v = 124775.0 - R_{D_2}/(n+0.082)^2$. Similar series with $v' = 1, 2$.						Q(1) lines (para- D_2)	(54)	
N=0 of D_2^+ :		{J=1 levels of $np\sigma \ ^1\Sigma_u^+$ ($n = 5...25, 36...45$, joining on to B, B', B'') ^b ; $v = 124745.5 - R_{D_2}/(n-0.203)^2$. Similar series with $v' = 1, 2$.						R(0) lines (ortho- D_2)	(54)	
$\bar{B} \ ^1\Sigma_u^+$		See $^1\text{H}_2$.								(48)(50)(60)
$D'' \ ^1\Pi_u \ 5p\pi \ 121227.5^d$		1648.6_8^d	33.63_8^{de}	15.13_3^{fg}	0.652_1^f	$[0.70_4]^f$	1.051_7	$D'' \leftarrow X, \ R \ 120497.0^d$		(14)(22)(54)
$D' \ ^1\Pi_u \ 4p\pi \ 118887.9^d$		1653.1_5^d	33.35^{dh}	15.04_1^{ig}	0.550_8^i	$[0.32_3]^i$	1.055_0	$D' \leftarrow X, \ R \ 118159.7^d$		(14)(22)(54)
$B'' \ ^1\Sigma_u^+ \ 4p\sigma \ 117970.7$		1563.0_2	35.41_6^j	13.68_5^g	0.384_2^k	$[0.02_4]$	1.106_0	$B'' \leftarrow X, \ R \ 117196.9$		(14)(22)(54)
$M \ ^1\Sigma_g^+ \ [114504.5]$		$v=0$ (?) only, fragmentary. [4.0]					$[2.0_6]$	$M \rightarrow B, \ R \ 22324.2$		(5)
$D \ ^1\Pi_u \ 3p\pi \ 113914.0$		1667.60	33.34_3^l	15.1_1^{mg}	0.54^n	0.5^n	1.05_3	$D \leftarrow X, \ R \ 113193.0^p$		(14)(22)
$I \ ^1\Pi_g \ 3d\pi \ 113081.5$		1600.14	39.42	14.739^{qr}	0.526^q	$[0.25]^q$	1.0657	$I \rightarrow B, \ V \ 21691.4^s$		(5)
$G \ ^1\Sigma_g^+ \ 3d\sigma \ (112893)$		$[1440.8]$	(perturbed) ^{tu}					$G \rightarrow B, \ R \ 21433.2$		(5)
$K \ (^1\Sigma_g^+) \ (112610)$		$[1660]$		$[6.6]$			$[1.5_9]$	$K \rightarrow B, \ (21260)^v$		(5)
$B' \ ^1\Sigma_u^+ \ 3p\sigma \ 111642.2^w$		1451.98	45.679^x	13.60_5^g	0.920^y	$[0.41_5]^z$	1.109_2	$B' \leftarrow X, \ R \ 110815.65$		(14)(22)(48)*

2H_2 , ^aCross sections for photoionization into the various vibrational levels of D_2^+ and the adjoining continuum (dissociative photoionization) observed by (24)(43) and calculated by (18)(26)(46)(51).

^bSee the remarks in ^bp.245 concerning the corresponding series of 1H_2 . Note, however, that an accurate representation using Fano's quantum defect theory has not yet been attempted for D_2 .

^cThis series of levels is obtained (54) from a Rydberg series of Q(1) lines whose limit is at 124715.2 cm^{-1} . A similar series of Q(2) lines with a limit at 124654 cm^{-1} converges to the $N=2$ level of D_2^+ ; also observed for $v=1$ and 2. These series, unlike $J=1$ of $np\sigma$, $^1\Sigma_u^+$ and $np\pi$, $^1\Pi_u^+$, are essentially unperturbed.

^dAverage of Π^+ and Π^- .

^e $\omega_e y_e = + 0.303_4$; $v = 0-5$.

^f $\gamma_e = + 0.0132_9$; constants refer to Π^- . For Π^+ (54) give $B_e = 16.19_8$, $\alpha_e = 0.618_8$, $\gamma_e = -0.0413_2$; $D_0 = 0.0078_5$.

^gRKR potential functions (21).

^h $\omega_e y_e = + 0.226$; a very small quartic term differs in sign for Π^+ and Π^- (54); $v = 0-7$.

ⁱ $\gamma_e = + 0.0050_3$; constants refer to Π^- . Π^+ is perturbed by $B''^1\Sigma_u^+$, particularly for $v=3$ and 7. After deperturbation, and excluding $v=2,4,8$, (54) obtain $B_v(\Pi^+, v=0-10) = 15.33_6 - 0.496_6(v+\frac{1}{2}) - 0.0048_9(v+\frac{1}{2})^2$; $D_0(\Pi^+) = 0.0075_6$.

^j $\omega_e y_e = + 0.084_3$, $\omega_e z_e = - 0.0136_4$; (22) gives slightly different constants. There are strong perturbations which make vibrational constants somewhat ambiguous.

^k $\gamma_e = - 0.0173_6$. Strong rotational perturbations in $v=4$, weaker ones in $v=3, 5$, and 9 caused by $D'^1\Pi_u^+$ (54).

$l + 0.1698(v+\frac{1}{2})^3 + 0.00296(v+\frac{1}{2})^4 - 0.000307(v+\frac{1}{2})^5$; the vibrational constants refer to the average of Π^+ and Π^- (22).

^mStrong predissociation for $v \geq 4$, not yet studied in detail but (36) observe line widths of 3.5 cm^{-1} for $J=2$, $v=4\dots7$ of Π^+ . (31) observe Ly_α of D in fluorescence as a consequence of predissociation and find a noticeable increase of predissociation when an electric field is applied (field-induced predissociation). Theoretical discussion (40).

ⁿ $\gamma_e = - 0.002$, D_v irregular; the rotational constants refer to Π^- .

^oFranck-Condon factors from electron energy loss spectra (28).

^pAverage of Π^+ and Π^- extrapolated to $J=0$. The Λ -type doubling for $v=0, J=1$ is 2.1_4 cm^{-1} with Π^+ above Π^- .

^qEffective constants for Π^- , strongly affected by l -uncoupling. See also I $^1\Pi_g$ of 1H_2 .

^rSee ^mp. 263.

^sRefers to the $J=1$ level of $^1\Pi^-$; the $J=1$ level of $^1\Pi^+$ lies 18.7 cm^{-1} higher.

^tZeeman effect in 0-0 band (9).

^uSee ⁱp. 263.

^vRefers to $J'=1$.

^wTakes account of Y_{00} in both upper and lower state. The Y'_{00} values for B, C, B' are $4.2, 2.2, 5.1 \text{ cm}^{-1}$, resp., but $Y_{00}(B')$ is uncertain; see comments regarding 1H_2 .

^x $\omega_e y_e = + 2.096$, $\omega_e z_e = - 0.294$, seven-level fit (48). (22) gives rather different constants based on a nine-level fit; his ninth level ($v=8$) disagrees strongly with that of (48).

^y $+ 0.102(v+\frac{1}{2})^2 - 0.0134(v+\frac{1}{2})^3$, seven-level fit (48).

^z $D_1 = 0.0037_1$, higher D_v values are irregular.

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State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^2\text{H}_2$ (continued)										
F } $1\Sigma^+_g\{2p\sigma^2(100931.2)^a$		[859.1] ^b		$B_6 = 3.5^c$			$r_6 = 2.2$	F→B, R $v_{60} = 13912.70$	(16)	
E } $1\Sigma^+_g\{2s\sigma$	100128.1	1784.42	48.10 ₅	16.369 ₆	0.6764	[0.54]	1.0112 ₄	E→B, V	8827.99	(16)
C } $1\Pi_u$	$2p\pi$ 100097.2 ^d	1729.92	34.917 ^e	15.673 ₁ ^f	0.5679 ^g	0.532 ^h	1.0334 ₆	C↔X, ⁱ R Werner b.	99409.18 ^j	(44)* (48)*
B } $1\Sigma^+_u$	$2p\sigma$ 91697.2 ^d	963.08	11.038 ^k	10.068 ₀ ^f	0.4198 ^l	0.40 ₃ ^m	1.2894 ₄	B↔X, ^{no} R Lyman b.	90633.79	(27)* (44)* (48)*
X } $1\Sigma^+_g$	$1s\sigma^2$ 0	3115.50	61.82 ^p	30.443 ₆ ^q	1.0786 ^r	1.141 ^s	0.74152	Field- and pressure-induced sp. ^t		(23) (17)(38)(49)
								Raman sp.		(11)
								Rf magn. reson. sp. ^u		(7)(10)(33) (35)

$^2\text{H}_2$: ^aFrom the observed v_{60} and the energy of $v=6$ above the (outer) minimum as calculated by (29); see $^1\text{H}_2$.

^bCalculated $\Delta G(\frac{1}{2})$ value of the outer minimum of the double-minimum state (29); see $^1\text{H}_2$. According to (29) the lowest level of the outer minimum is 9190.1 cm^{-1} above B $1\Sigma_u^+(v=0)$, but the $v=0\dots 5$ levels have not yet been observed. The $v=6$ level lies just below the potential maximum.

^cVibrational numbering of (29). The D_6 value is large and negative. Higher vibrational levels lie above the potential maximum and have larger B_v values (e.g. B_{12}

= 5.688) corresponding to the fact that for these levels the vibrational motion covers both minima of the E,F state. A few rotational levels of $v=4$ have been observed.

^dSee ^wp. 265. T_e of C $1\Pi_u$ and $v_{00}(\text{C-X})$ both exclude $-B\Lambda^2$. ^e $w_e y_e = +0.2612$, $w_e z_e = -0.00946$; the zero-point energy ($Y_{00} = 2.2$ included) is 858.4₆ cm^{-1} . The eight-level fit refers to Π^- (48). All vibrational levels up to $v=19$ have been observed. The last level lies 50 cm^{-1} above the dissociation limit confirming the theoretical prediction (13) of a maximum in the potential function.

^fRKR potential functions (21).

$^2\text{H}_2$ (continued):

$^g + 0.00419(v+\frac{1}{2})^2 - 0.00010_1(v+\frac{1}{2})^3$, eight-level fit referring to $^1\Pi_u^-$ (48). Several of the $^1\Pi_u^+$ levels are strongly perturbed by B $^1\Sigma_u^+$.

$^h - 0.000216(v+\frac{1}{2}) + 0.000011(v+\frac{1}{2})^2$.

i Franck-Condon factors from electron energy loss spectra (28). Theoretical band oscillator strengths, transition probabilities and photodissociation cross sections (30).

j Excludes $-B\Lambda^2$.

$^k + 0.4109(v+\frac{1}{2})^3 - 0.0370(v+\frac{1}{2})^4 + 0.00154(v+\frac{1}{2})^5$, the zero-point energy ($Y_{00} = 4.2$ included) is 483.0_3 cm^{-1} ; eight-level fit (48). All vibrational levels up to $v=51$ have been observed.

$^l + 0.0296(v+\frac{1}{2})^2 - 0.0015(v+\frac{1}{2})^3$, eight-level fit (48).

$^m - 0.000320(v+\frac{1}{2}) + 0.000013(v+\frac{1}{2})^2$.

n Selective enhancements of $v'=7$ and 9 in Ar- D_2 mixtures studied by (20). Experimental Franck-Condon factors (28), calculated (18a). Theoretical band oscillator strengths, transition probabilities, and photodissociation cross sections (30).

o Continuous component of B-X (corresponding to the continuum of X $^1\Sigma_g^+$) observed by (32).

$^p \omega_e y_e = + 0.562$, $\omega_e z_e = - 0.0228_6$; the zero-point energy ($Y_{00} = 4.1_3$ included) is 1546.4_9 cm^{-1} . Data from the Raman measurements of (11) and the field-induced spectrum of (23) have been combined with the somewhat less accurate VUV results in the least-squares solution (10-level fit) for the vibrational and rotational constants (44). All vibrational levels have been observed, the last one, $v=21$, being only 2.1 cm^{-1} below the dissociation limit (44). Theoretical values for all bound and quasi-bound

levels are given by (37); see also (52). For a discussion of the small differences obs.-calc. see (39)(44)(55).

q According to (8) the hyperfine levels $F=1$ and 2 for $v=0, J=1$ (para- D_2) are 0.6609×10^{-5} and $0.4669 \times 10^{-5} \text{ cm}^{-1}$ below the $F=0$ component.

$^r + 0.01265(v+\frac{1}{2})^2 - 0.00069(v+\frac{1}{2})^3$; see P. As for $^1\text{H}_2$ the B_v curve has a slightly negative curvature at low v .

$^s - 0.00022_4(v+\frac{1}{2}) - + \dots$, from the data of (11)(23)(44).

t 1-0 and 2-0 bands.

u Nuclear spectrum (7); the rotational spectrum gives the rotational magnetic moment for $J=1$: $0.44288 \mu_N$ (10). (35) determine spin-rotation and quadrupole interaction constants for $J=1,2$ and derive the quadrupole moment of D. Polarizability anisotropy $\alpha_{||} - \alpha_{\perp} = 0.289_7 \text{ \AA}^3$ (33).

(1) See ref. (5) of $^1\text{H}_2$.

(2) See ref. (6) of $^1\text{H}_2$.

(3) See ref. (7) of $^1\text{H}_2$.

(4) Jeppesen, PR 49, 797 (1936).

(5) See ref. (10) of $^1\text{H}_2$.

(6) See ref. (15a) of $^1\text{H}_2$.

(7) See ref. (17) of $^1\text{H}_2$.

(8) See ref. (16) of $^1\text{H}_2$.

(9) Dieke, JPR 15, 393 (1954).

(10) Ramsey, "Molecular Beams", p. 238. Clarendon Press, Oxford (1956).

(11) See ref. (23) of $^1\text{H}_2$.

(12) See ref. (12) of $^1\text{H}_2^2\text{H}$.

(13) See ref. (43) of $^1\text{H}_2$.

(14) See ref. (46) of $^1\text{H}_2$.

(continued p. 269)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$2\text{H}^3\text{H}$		$\mu = 1.20764393$		$D_0^0 = (4.5727_1) \text{ eV}^a$		$\text{I.P.} = (15.4749_6) \text{ eV}^b$				NOV 1976
a	$3\Sigma_g^+ 2s\sigma$ (95961.8) ^c							(a-X)	(95404.6) ^d	
C	$1\Pi_u 2p\pi$ (100098.4) ^c							(C-X)	(99470.0) ^d	
B	$1\Sigma_u^+ 2p\sigma$ (91696.7) ^c							(B-X)	(90724.9) ^d	
X	$1\Sigma_g^+ 1s\sigma^2$ 0	2845.5_2^e	51.38_6^e	25.395^e	0.8221^e	0.809^f	(0.74142)			(1)(3)

$2\text{H}^3\text{H}$: $a_{36881.1} \text{ cm}^{-1}$, calculated from ab initio potential function (5); non-adiabatic corrections which are certainly less than $+0.2 \text{ cm}^{-1}$ and Lamb shift corrections ($\approx -0.2 \text{ cm}^{-1}$) are not included. No observed value is available yet.

^bFrom the theoretical $D_0^0(\text{DT})$ and $D_0^0(\text{DT}^+)$ values and I.P.(D).

^cFrom the T_e values of H_2 and D_2 assuming that the electronic isotope shift is proportional to $(1 - \mu_{\text{H}_2}/\mu_{\text{DT}})$.

^dFrom T_e and the zero-point energy calculated by (4).

^eCalculated by (3) from the potential function of (2) and based on $v=0\dots 3$ only; $w_e v_e = +0.336$, $y_e = +0.0087$,

$Y_{00} = 3.4$. Slightly different numbers were obtained by (1) from the constants of H_2 by using isotope relations.

^fCalculated by (1) from the constants of H_2 using isotope relations; $\beta_e = -0.000114$.

(1) Jones, JCP 17, 1062 (1949).

(2) See ref. (43) of $^1\text{H}_2$.

(3) See ref. (5) of $^1\text{H}^3\text{H}$.

(4) See ref. (67) of $^1\text{H}_2$.

(5) See ref. (70) of $^1\text{H}_2$.

$^2\text{H}_2$ (continued):

- (15) See ref. (47) of $^1\text{H}_2$.
- (16) Dieke, Cunningham, JMS 18, 288 (1965).
- (17) Watanabe, Welsh, CJP 43, 818 (1965).
- (18) See ref. (50) of $^1\text{H}_2$.
- (18a) See ref. (51) of $^1\text{H}_2$.
- (19) Fowler, Holzberlein, JCP 45, 1123 (1966).
- (20) See ref. (15) of $^1\text{H}^2\text{H}$.
- (21) See ref. (72) of $^1\text{H}_2$.
- (22) See ref. (73) of $^1\text{H}_2$.
- (23) See ref. (74) of $^1\text{H}_2$.
- (24) See ref. (68) of $^1\text{H}_2$.
- (25) See ref. (70) of $^1\text{H}_2$.
- (26) See ref. (71) of $^1\text{H}_2$.
- (27) See ref. (77) of $^1\text{H}_2$.
- (28) See ref. (83) of $^1\text{H}_2$.
- (29) See ref. (86) of $^1\text{H}_2$.
- (30) See ref. (80)(90)(91) of $^1\text{H}_2$.
- (31) See ref. (92) of $^1\text{H}_2$.
- (32) See ref. (94) of $^1\text{H}_2$.
- (33) English, MacAdam, PRL 24, 555 (1970).
- (34) See ref. (95) of $^1\text{H}_2$.
- (35) Code, Ramsey, PR A 4, 1945 (1971).
- (36) See ref. (103) of $^1\text{H}_2$.
- (37) See ref. (31) of $^1\text{H}^2\text{H}$.
- (38) Reddy, Kuo, JMS 37, 327 (1971).
- (39) See ref. (115) of $^1\text{H}_2$.
- (40) See ref. (112) of $^1\text{H}_2$.
- (41) Herzberg, Science 177, 123 (1972).
- (42) See ref. (111) of $^1\text{H}_2$.
- (42a) See ref. (117) of $^1\text{H}_2$.
- (43) See ref. (37) of $^1\text{H}^2\text{H}$.
- (44) Bredohl, Herzberg, CJP 51, 867 (1973).
- (45) Freund, Miller, JCP 59, 4073 (1973).
- (46) See ref. (39) of $^1\text{H}^2\text{H}$.
- (47) See ref. (127) of $^1\text{H}_2$.
- (48) See ref. (129) of $^1\text{H}_2$.
- (49) Russell, Reddy, Cho, JMS 52, 72 (1974).
- (50) See ref. (155) of $^1\text{H}_2$.
- (51) See ref. (147) of $^1\text{H}_2$.
- (52) See ref. (153) of $^1\text{H}_2$.
- (53) Le Roy, Barwell, CJP 53, 1983 (1975).
- (54) Takezawa, Tanaka, JMS 54, 379 (1975).
- (55) See ref. (158) of $^1\text{H}_2$.
- (56) Jost, Lombardi, Derouard, Freund, Miller, Zeg CPL 37, 507 (1976).
- (57) Miller, Freund, Zegarski, JCP 64, 1842 (1976).
- (58) Bunker, unpublished.
- (59) Herzberg, unpublished.
- (60) Kolos, JMS 62, 429 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^3\text{H}_2$		$\mu = 1.50802486$		$D_0^0 = (4.59097) \text{ eV}^a$		$\text{I.P.} = (15.4867_0) \text{ eV}^b$				NOV 1976
n $^3\Pi_u 5p\pi$ (120984.3)		1348.89	22.52	10.021	0.294	0.22	1.0562	n \rightarrow a, R	24923.03	(2)
k $^3\Pi_u 4p\pi$ (118403.2)		1355.39	22.026 ^c	10.053	0.296	0.22	1.0545	k \rightarrow a, R	22345.34	(2)
f $^3\Sigma_u^+ 4p\sigma$ (116653)		[1278]		9.90	0.30		1.063	f \rightarrow a, R	20561.9	(2)
d $^3\Pi_u 3p\pi$ (112736.0)		1372.11	22.135 ^d	10.150 ^e	0.3050 ^e	0.217 ^f	1.0494	d \rightarrow a, R Fulcher b.	16686.4 ₄	(1)
e $^3\Sigma_u^+ 3p\sigma$ (107770.8)		1272.28	23.03 ^g	9.2056	0.2803 ^h	0.1887 ⁱ	1.1019 ₇	e \rightarrow a, R	11671.06	(3)
a $^3\Sigma_g^+ 2s\sigma$ (95965.4) ^j		1541.57	24.47 ^k	11.4374	0.3258 ^l		0.98862	(a - X)	(95464.4) ^m	
b $^3\Sigma_u^+ 2p\sigma$		Repulsive state, lower state of T_2 continuum.						a \rightarrow b		
F } $^1\Sigma_g^+ \{ 2p\sigma^2$ (100935.9) ⁿ		[706.0] ^o		$B_8 = 2.5_0^p$			$r_8 = 2.11$	F \rightarrow B, R	$v_{80} = 14302.50^q$	(4)
E } $^1\Sigma_g^+ \{ 2s\sigma$ (100136.7)		1454.18	30.52	10.9306	0.3659	0.2403	1.0112 ₈	E \rightarrow B, V	8765.40	(4)
C $^1\Pi_u 2p\pi$ (100099.7) ^j								(C - X)	(99536.9) ^r	
B $^1\Sigma_u^+ 2p\sigma$ (91696.3) ^j		787.28 ^s	7.013 ^s	6.716 ^t	0.207 ₆ ^t	0.17 ₃ ^t	1.290 ₁	(B - X)	(90825.0) ^u	
X $^1\Sigma_g^+ 1s\sigma^2$	0	2546.4 ₇ ^v	41.23 ^v	20.335 ^v	0.5887 ^w		(0.74142)			(6)

$^3\text{H}_2$: $a_{37028.4 \text{ cm}^{-1}}$, calculated from ab initio potential function (8); non-adiabatic corrections which are certainly less than $+0.2 \text{ cm}^{-1}$ and Lamb shift corrections ($\approx -0.2 \text{ cm}^{-1}$) are not included. No observed value is available yet.

^bFrom the theoretical values of $D_0^0(T_2)$ and $D_0^0(T_2^+)$, and I.P.(T).

^c $w_e y_e = +0.133$.

^d $w_e y_e = +0.159$, $w_e z_e = -0.002$.

^e $r_e = +0.0038$. The rotational constants refer to $^3\Pi^-$; $^3\Pi^+$ is perturbed. The Λ -type doubling is somewhat irregular.

^f $\beta_e = -0.000065$.

^g $w_e y_e = +0.170$, $w_e z_e = -0.0204$.

^h $r_e = -0.00156$.

$^3\text{H}_2$ (continued):

ⁱ $\beta_e = -0.000045$.

^jFrom the T_e values of H_2 and D_2 assuming that the electronic isotope shift is proportional to $(1 - \mu_{\text{H}_2}/\mu_{\text{T}_2})$.

^k $\omega_e v_e = +0.312$, $\omega_e z_e = -0.016$.

^l $\gamma_e = +0.00273$.

^mFrom T_e assuming $Y_{00}(a^3\Sigma_g^+) = 0$ but taking account of Y_{00} in the ground state $X^1\Sigma_g^+$ (see ^v).

ⁿFrom the observed v_{80} and the energy of $v=8$ above the outer minimum of the E,F double-minimum state as calculated by (9).

^oCalculated $\Delta G(\frac{1}{2})$ value for the outer minimum (9).

^pVibrational numbering of (9). The D_8 value is large and negative. For higher vibrational levels (above the potential maximum) B_v is larger, e.g. (4) give $B_{13} = 3.892$, and $D_{13} = 0.00109$ has the normal sign, in agreement with the fact that for these levels the vibrational motion covers both minima of the E,F state. $v=0\dots7$ levels not yet observed.

^qAccording to (9) the lowest level of the outer minimum is expected at 9204.5 cm^{-1} above $B^1\Sigma_u^+(v=0)$. The $v=8$ level lies just below the potential maximum.

^rFrom T_e and the zero-point energy calculated by (7).

^sFrom the $R(0)$ lines in the E,F-B system (4); $\omega_e v_e = +0.0912$. The zero-point energy ($Y_{00} = 2.6$ included) is 394.46 cm^{-1} .

^tFrom combination differences formed from the data on E,F-B (4); $\gamma_e = +0.0072$, $\beta_e = -0.0008$.

^uFrom the calculated T_e and the zero-point energies as given in ^s and ^v.

^vCalculated by (6) from the potential function of (5) and based on $v=0\dots3$ only; experimental values are not available. $\omega_e v_e = +0.258$; the zero-point energy ($Y_{00} = 2.8$ included) is 1265.74 cm^{-1} .

^w $+0.0053(v+\frac{1}{2})^2 - 0.00018(v+\frac{1}{2})^3$; see ^v.

(1) See ref. (1) of $^1\text{H}^3\text{H}$.

(2) See ref. (15a) of $^1\text{H}_2$.

(3) See ref. (3) of $^1\text{H}^3\text{H}$.

(4) See ref. (16) of $^2\text{H}_2$.

(5) See ref. (43) of $^1\text{H}_2$.

(6) See ref. (5) of $^1\text{H}^3\text{H}$.

(7) See ref. (67) of $^1\text{H}_2$.

(8) See ref. (70) of $^1\text{H}_2$.

(9) See ref. (86) of $^1\text{H}_2$.

(10) See ref. (152) of $^1\text{H}_2$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
<div><div>H_2^+</div><div>$\mu = 0.50377547$<div>$D_0^0 = 2.65078 \text{ eV}^a$</div></div><div>Several other predicted excited states, mostly repulsive.^b</div></div>											
C	$2\Pi_u$	2p π (102696. ₇) ^c	(266.0 ₁)	(6.45 ₄)	(1.899)	(0.075 ₈)	(0.039)	(4.19 ₈)	(C-B)	(8806.3) ^c	(27)
B	$2\Sigma_g^+$	3d σ (93804. ₅) ^c	(437.1 ₅)	(5.24 ₇)	(1.530)	(0.031 ₂)	(0.0075)	(4.67 ₇)	(B-X)	(92877. ₄)	(27)
A	$2\Sigma_u^+$	2p σ	Repulsive state. ^d					A \leftarrow X		(11)	
X	$2\Sigma_g^+$	1s σ 0	2321. ₇ ^e	66.2 ^e	30.2 ₁ ^{efg}	1.68 ₅ ^e	e	1.052 ^h	Spin reorientation sp. ⁱ		(13)
<div><div>H_2H^+</div><div>$\mu = 0.67155901$<div>$D_0^0 = 2.66771 \text{ eV}^a$</div></div><div>[1913.1]^b</div></div>											
X	$2\Sigma_g^+$	1s σ 0			(22.45 ₂) ^c	(1.00 ₁) ^c	(1.1) ^c	(1.057)	Rotation-vibration sp. ^d		(5)
<div><div>H_3H^+</div><div>$\mu = 0.75523263$<div>$D_0^0 = (2.67401_7) \text{ eV}^e$</div></div><div>[(1809.234)]^e</div></div>											
X	$2\Sigma_g^+$	1s σ 0									(NOV 1976 A)

$^1\text{H}_2^+$: ^aExperimental value derived from $D_0^0(\text{H}_2)$ and I.P.(H_2) (21). The latest theoretical value [non-adiabatic calculation (25), and including relativistic and Lamb shift corrections] is 2.65073 eV; see also (7)(14).

^bElectronic wavefunctions and energies are given by (2) where references to earlier literature may be found.

^cData for these two states are entirely theoretical [adiabatic approximation (27); see also (19)]. $v_{00}(\text{C-B})$ refers to $N=1$ of C $2\Pi_u$ and $N=0$ of B $2\Sigma_g^+$; see Table VI of (27). Beckel (lecture at Columbus 1976) gives 8803.9₀.

^dObserved in the photodissociation of H_2^+ (11)(13) and in the photoelectron spectrum of H_2 (22); the direct transition from the X $1\Sigma_g^+$ ground state causes a shoulder in the absorption spectrum of H_2 near 380 \AA . Of recent ab initio

calculations of the potential function the most detailed seems to be that of (4). This state has a small van der Waals minimum ($D_0 = 3.4 \text{ cm}^{-1}$) at 6.64 \AA (16).

^eFrom Rydberg series limits of H_2 (21); $\Delta G(\frac{1}{2}) = 2191.2$, $w_e v_e = +0.6$, $\gamma_e = +0.041_2$. Similar constants (and $D_e = 0.018$) were obtained (1) by extrapolation from low members of the series $np^3\Pi$ ($n=2-5$). Higher vibrational levels and their B_v values have been derived from photoelectron spectra (8)(17). See also ¹.

^fFor two recent ab initio calculations of the potential function s. (4)(26); relativistic corrections (15), Lamb shift corrections (12)(14), non-adiabatic corrections (25). Rotational and vibrational levels up to $v=18$ from ab initio calculations in (5)(7)(18)(26), incl. quasi-bound levels.

$^1\text{H}_2^+$ (continued),

^gFranck-Condon factors for photoionization of H_2 (3)(6) (10). Effect of r-dependence of the transition moment (24). Experimental cross sections (9)(23).

^hThe most recent theoretical value (20) is 1.0569 Å.

ⁱObserved for $N=1$ and $N=2$ of $v=4\dots 8$. For $v=4, N=2$ the spin splitting is 0.0027059 cm^{-1} ; for odd N the hyperfine structure due to the proton spins is superposed which gives a much larger splitting. The strongest of the observed five transitions for $v=4, N=1$ occurs at 0.0423810 cm^{-1} ; the extrapolated wavenumber for $v=0, N=1$ is 0.046842 .

(1) See ref. (15a) of $^1\text{H}_2$.

(2) Bates, Ledsham, Stewart, PTRSL A 246, 215 (1953).

(3) Halmann, Laulicht, JCP 43, 1503 (1965).

(4) Peek, JCP 43, 3004 (1965); see also Sandia Corp. Rep. No. SC-RR-65-77 (1965) and supplement.

(5) Wind, JCP 43, 2956 (1965).

(6) See ref. (50) of $^1\text{H}_2$.

(7) Hunter, Pritchard, JCP 46, 2153 (1967).

(8) Siegbahn, Nordling, Fahlman, Nordberg, Hamrin, Hedman, Johansson, Bergmark, Karlsson, Lindgren, Lindberg, "ESCA - Atomic, Molecular and Solid State Structure Studied by Means of Electron Spectroscopy", p. 208f.; NARSSU (IV) 20 (Uppsala, 1967).

(9) Spohr, von Puttkamer, ZN 22 a, 705 (1967).

(10) See ref. (75) of $^1\text{H}_2$.

(11) Richardson, Jefferts, Dehmelt, PR 165, 80 (1968).

(12) Gersten, JCP 51, 3181 (1969).

(13) Jefferts, PRL 23, 1476 (1969).

(14) See ref. (79) of $^1\text{H}_2$.

(15) Luke, Hunter, McEachran, Cohen, JCP 50, 1644 (1969).

(16) Peek, JCP 50, 4595 (1969).

(17) Åsbrink, CPL 7, 549 (1970).

(18) Beckel, Hansen, Peek, JCP 53, 3681 (1970).

$^1\text{H}^2\text{H}^+$; $^1\text{H}^3\text{H}^+$,

^aFrom $\text{D}_0^0(\text{HD})$, I.P.(HD), and I.P.(H). A second dissociation limit corresponding to $\text{H}+\text{D}^+$ is only 0.00370 eV higher. The theoretical value for $\text{D}_0^0(\text{HD}^+)$ is 2.66767_9 eV (3)(6).

^b $\Delta G(3/2) = 1816.7$, $\Delta G(5/2) = 1723.7$; from Rydberg series of HD (1). *Ab initio* calculations (6) give $\Delta G(1/2) = 1913.005$.

^cAll bound rotational and vibrational levels derived from the *ab initio* potential function in the adiabatic approximation are listed by (4); see also (2). The rotational constants in the table are based on these calculated levels (4) using $v=0$ and 1 only.

^dSeveral lines of the 1-0, 2-1, 3-2 infrared bands have been observed and measured with high accuracy by (5) but there are not enough lines to obtain "observed" values for the rotational constants. The lines show a splitting of 0.0010 cm^{-1} corresponding to the difference in spin splitting in the upper and lower state.

^eTheoretical value (6).

(1) See ref. (36) of $^1\text{H}^2\text{H}$.

(2) Bishop, Wetmore, JMS 46, 502 (1973).

(3) See ref. (25) of $^1\text{H}_2^+$.

(4) See ref. (26) of $^1\text{H}_2^+$.

(5) Wing, Ruff, Lamb, Spezeski, PRL 36, 1488 (1976).

(6) Bishop, PRL 37, 484 (1976).

(19) Kroll, JMS 35, 436 (1970).

(20) Shaad, Hicks, JCP 53, 851 (1970).

(21) See ref. (114) of $^1\text{H}_2$.

(22) Samson, CPL 12, 625 (1972).

(23) See ref. (37) of $^1\text{H}^2\text{H}$.

(24) See ref. (39) of $^1\text{H}^2\text{H}$.

(25) Bishop, MP 28, 1397 (1974).

(26) Hunter, Yau, Pritchard, ADNDT 14, 11 (1974).

(27) Bishop, Shih, Beckel, Wu, Peek, JCP 63, 4836 (1975).

2H_2^+ , $2\text{H}^3\text{H}^+$, 3H_2^+ ;

^aFrom $D_0^0(D_2)$ and I.P.(D_2); theoretical value 2.69192 eV (8).

^bData for these two states are entirely theoretical (7).

^c $w_{ey_e} = -0.027$.

^d $r_e = -0.0003$.

^e $w_{ey_e} = +0.011$.

^f $\Delta G(3/2) = 1512.1$; from Rydberg series of D_2 (10). Corresponding theoretical values 1577.15, 1512.47 [adiabatic approximation (9)]. Higher vibrational levels [observed in photoionization (6) and photoelectron (5) spectra] and rotational levels, incl. quasi-bound levels, calculated by (4)(9). Franck-Condon factors for photoionization of D_2 from $X^1\Sigma_g^+$ calculated by (2)(3) and measured by (5)(6).

^gExtrapolated (1) from low members of the Rydberg series $np^3\Pi$ ($n=2\dots 6$) of D_2 . See also ^f.

^hTheoretical value (11).

ⁱCalculated from the Born-Oppenheimer pot. function and the adiabatic corrections (scaled down for T_2^+) given by (12).

^jExtrapolated (1) from low members of the Rydberg series $np^3\Pi$ ($n=2\dots 5$) of T_2 .

(1) See ref. (15a) of 1H_2 .

(2) See ref. (3) of 1H_2^+ .

(3) See ref. (50) of 1H_2 .

(4) See ref. (7) of 1H_2^+ .

(5) See ref. (9) of 1H_2^+ .

(6) See ref. (68) of 1H_2 .

(7) See ref. (19) of 1H_2^+ .

(8) See ref. (25) of 1H_2^+ .

(9) See ref. (26) of 1H_2^+ .

(10) See ref. (54) of 2H_2 .

(11) See ref. (6) of $1\text{H}^2\text{H}^+$, $1\text{H}^3\text{H}^+$.

(12) Bishop, Wetmore, MP 26, 145 (1973).

1H_2^- ,

^aTwo progressions of resonances (series "f" and "g") proceeding across the ionization threshold of H_2^+ . Higher members correlate with structure previously observed in photoionization of H_2 .

^bEnergies in eV above $X^1\Sigma_g^+(v=0)$ of H_2 , all obtained as resonances in electron scattering experiments. The value for $B^2\Sigma_g^+$ is extrapolated from $v=2$.

^cFrom resolved rotational structure of the resonances (2).

^dFrom a fit of calculated to observed excitation cross sections (2); for $D^2\Sigma_g^+$ in good agreement with the value obtained from the observed rotational structure.

^eThe progressions of resonances attributed to B, C, D are normally referred to as series "b", "c", "a", resp..

^fAssignment according to (6); (2) favour $1s5s\sigma^2p\pi$, $2\Pi_u$.

^gPossible parent state $B^1\Sigma_u^+$.

^hThe potential function is well defined only outside the potential well of H_2 [see, however, (1)]; its asymptote lies 0.75421 eV below that of $\text{H}_2 X^1\Sigma_g^+$. The lifetime against preionization is estimated to be 10^{-15} s corresponding to a width of 1 eV. The ground state of H_2^- causes a broad resonance in the scattering of low energy electrons by H_2 and shows up both in the formation of H^- by dissociative attachment and in the vibrational excitation of H_2 .

(1) Eliezer, Taylor, Williams, JCP 47, 2165 (1967).

(2) Comer, Read, JP B 4, 368 (1971); Joyez, Comer, Read, JP B 6, 2427 (1973).

(3) Schulz, RMP 45, 423 (1973).

(4) Spence, JP B 7, L87 (1974).

(5) Schowengerdt, Golden, PR A 11, 160 (1975).

(6) Chang, PR A 12, 2399 (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^1\text{H}^8\text{Br}$								$\mu = 0.99542702$ $D_0^0 = 3.758 \text{ eV}^a$ I.P. = 11.67 eV^b		DEC 1976 A
Numerous absorption bands above 114000 cm^{-1} , tentatively assigned to higher members of two Rydberg series starting with L and M and converging to $A^2\Sigma^+$ of HBr^+ ; I.P. [$A^2\Sigma^+, v=0$] = 123373 cm^{-1} (15.296_4 eV).								(43)		
M ($^1\Sigma^+$)	(109473)	[1308]	$v=0\dots 4$ observed. Assigned as $4p\sigma 4p\pi^4 6s\sigma^c$					M \leftarrow X,	108814	(43)*
L ($^1\Sigma^+, ^1\Pi$)	(104201)	[1262]	$v=0\dots 3$ observed. Assigned as $4p\sigma 4p\pi^4 5p\sigma$ and/or $5p\pi^c$					L \leftarrow X,	103519	(43)*
Further absorption bands of doubtful assignment between 75200 and 83600 cm^{-1} .								(13)(15)		
K ^d	1 (83902)	(2518) ^e	[8.195]			[22.0]	[1.437 ₅]	K \leftarrow X, R	83847.9^f Z	(15)
J ^d	1 (81243)	(2502) ^e	[8.02 ₇] ^g			[3.6 ₁]	[1.453]	J \leftarrow X, R	81180.7^h Z	(13)*
I ^d	1 (80436)	(2525) ^e	[8.16 ₉] ⁱ			[10.4]	[1.440]	I \leftarrow X, R	80385.6^j Z	(13)*
g ($^3\Sigma^-$) ⁺ t	[79253.2]		[7.6 ₃] ^k			[-17]	[1.49]	g \leftarrow X, R	77940.0 Z	(13)* (36)*
F $^1\Delta$	t [78322.3]		[8.20]				[1.43 ₇]	F \leftarrow X, R	77009.1 Z	(36)*
f ₁ $^3\Delta_1$	t (76814)	[2299.7] Z	8.02 ₇	0.21 ₃			1.453	f ₁ \leftarrow X, R	76650.9 Z	(13)(36)*
D $^1\Pi$	u (76310)	[2405.5] Z	8.12 ₅	0.21			1.444	D \leftarrow X, R	76199.4 Z	(13)* (36)*
d ₀ $^3\Pi_0$	u (76193)	[2418.5] Z	[7.624] ^l	(0.32)			[1.490 ₄]	d ₀ \leftarrow X, R	76088.8 Z	(13)(36)*
E ($^1\Sigma^+$) ⁺ t	[76691]		[7.34] ^m				[1.51 ₉]	E \leftarrow X, R	75378	(36)
v $^1\Sigma^+$	n (75800)	(790)	Bands in emission above 46500 cm^{-1} , in absorption above 75700 . Incomplete analysis.					V \leftrightarrow X, ^o R	(74900)	(14)(36)*
f ₂ $^3\Delta_2$	t [75533.8]		[8.67 ₅] ^p			[16.5] ^p	[1.397]	f ₂ \leftarrow X, R	74220.6 Z	(13)(36)*
f ₃ $^3\Delta_3$	t [75403.1]	Weak transition.	[7.41]			[-7.6]	[1.51 ₂]	f ₃ \leftarrow X, R	74089.9 Z	(36)*
e $^3\Sigma^+$	t [75053]	Very diffuse, unresolved band.						e \leftarrow X, R	73740	(36)
d ₁ $^3\Pi_1$	u [74855]	Diffuse band, rotational structure unresolved.						d ₁ \leftarrow X, R	73542	(13)(36)
d ₂ $^3\Pi_2$	u [74753]	Diffuse band, rotational structure unresolved.						d ₂ \leftarrow X, R	73440	(13)(36)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^1\text{H}^{81}\text{Br}$ (continued)										
$c \ ^1\Pi$	$v \ 70578$	2552	$Z \ 52$	7.89	0.30		1.46 ₅	$C \leftarrow X, ^q$	$R \ 70527.6 \ Z$	(13)(32)*
	$o^+ \ v \ (68998)$	[2452]		[7.99 ₆] ^r			[1.455]	R	$68911.2 \ Z$	
$b_0 \ ^3\Pi_0$	$o^- \ v \ (68991)$							$b_0 \leftarrow X,$	$R \ 68904^s \ H$	(13)(32)*
$b_1 \ ^3\Pi_1$	$v \ (67180)$	[2444.2]	Z	8.14 ₈ ^r	0.29 ₂		1.442	$b_1 \leftarrow X,$	$R \ 67088.4 \ Z$	(13)* (32)*
$b_2 \ ^3\Pi_2$	$v \ [67663.0]$			[7.80 ₅] ^r			[1.473]	$b_2 \leftarrow X,$	$R \ 66349.8 \ Z$	(13)(32)*

¹HBr: ^aFrom D₀⁰(H₂), D₀⁰(Br₂), and ΔH_{f0} (HBr; from gaseous H₂, Br₂).

^bAverage value from photoionization (10) and photoelectron spectra (23)(29); refers to X ² $\Pi_{3/2}$ of the ion. A more recent paper (39) gives 11.64₅ eV.

^cStrongly broadened by preionization; estimated lifetime against preionization 9.5×10^{-15} s (46).

^dI, J, K correspond to absorption bands with clear analogues in DBr.

^eFrom the observed HBr-DBr isotope shift assuming that the observed bands are 0-0 bands.

^fBand [37] of (15).

^g Ω -type doubling, $\Delta v_{ef} = + 0.14_2 \times J(J+1) - \dots$; B and D represent average values.

^hBand [28] of (13). Sharp P, Q, R branches; the Q levels appear to be predissociated for $J \geq 14$.

ⁱFrom R, P branches. $\Delta v_{ef} = - 0.041 \times J(J+1)$.

^jBand [26] of (13).

^kPerturbed at high J.

^lSlightly diffuse lines.

^mPerturbed.

ⁿDerived from H⁺ + Br⁻; configuration ... $\sigma^4 \pi^4 \sigma^*$.

^oHeavily perturbed extensive band system. Absorption lines above 75923 cm⁻¹ are diffuse. B' varies irregularly between 3.4 and 4.5 cm⁻¹.

^pAverage values for the two Ω -type doubling components.

^qVery strong absorption, lines are diffuse.

^rDiffuse rotational structure.

^sDiffuse Q head.

^tConfiguration ... $\sigma^2 \pi^3 5p\pi$.

^uConfiguration ... $\sigma^2 \pi^3 5p\sigma$.

^vConfiguration ... $\sigma^2 \pi^3 5s\sigma$.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
¹ H ⁸¹ Br (continued)										
A (¹ Π)	^w	Continuous absorption starting at ~ 35000 with maximum at 56400 cm^{-1} .						A \leftarrow X	(1)(2)(4)(5) (28)	
X (¹ Σ^+)	0	2648.975^x	z 45.217_5^y	8.46488_4^x	0.23328^z	$3.457_5^{a'}$	1.41443_5	Rot.-vibr. sp. $b'c'$ Rotation spectrum $d'c'$ Raman sp. e' Mol. beam el. reson. f'	(21) (8)(17)(31) (45) (42)	

¹HBr (continued):

^wConfiguration ... $\sigma^2\pi^3\sigma^*$.

^xThese are Y_{10} and Y_{01} values; applying Dunham corrections (21) obtain $\omega_e = 2649.21_5$, $B_e = 8.46506_5$. Additional corrections (adiabatic, non-adiabatic) are discussed by (38). The microwave B_0 value of (17) was included in the evaluation of B_e . See also $b'f'$.

^y $\omega_e y_e = -0.0029$.

^z $+0.000873_5(v+\frac{1}{2})^2 - 0.000120(v+\frac{1}{2})^3$.

^{a'} $-0.039_7 \times 10^{-4}(v+\frac{1}{2}) + 0.0038(v+\frac{1}{2})^2$;

$H_v = 7.63 \times 10^{-9} - 0.55 \times 10^{-9}(v+\frac{1}{2})$.

^{b'}In absorption the 1-0, 2-0, 3-0, 3-1, 4-0, 5-0, 6-0 bands have been studied (6)(7)(12)(21)(41); in emission 1-0, 2-1, 3-2, 4-3 (11)(20). The constants in the table are from (21), those of (20)(41) are very similar and of comparable accuracy. See also (47). Absolute intensities have been measured (16)(18)(30)(33) and the dipole moment function has been

calculated; (40) give for $H^{79}\text{Br}$ [$D, \text{\AA}$]: $\mu_{el}(r) = +0.788 + 0.315(r-r_e) + 0.575(r-r_e)^2$; see also (24)(34)(37).

^{c'}For observations and measurements of pressure-induced bands and pure rotation lines ($\Delta J=2$) see (22)(27). The pressure broadening of the lines has been studied by (16)(25).

^{d'}Absolute intensities have been measured by (19).

^{e'}Raman cross sections in gaseous HBr.

^{f'}The following constants (as well as corresponding values for $H^{79}\text{Br}$) are given in (42):

- $\mu_{el}(v=0, J=1) = 0.8265 D$ [in a later paper (44) derive $0.8282 D$ from Stark effect of rotation spectrum];

- quadrupole and other hyperfine coupling constants;

- $g_J = 0.3712$.

These constants supersede earlier values of (9)(17)(26)(31)(35).

¹HBr (continued):

- (1) Bates, Halford, Anderson, JCP 3, 531 (1935).
- (2) Goodeve, Taylor, PRS A 152, 221 (1935).
- (3) Price, PRS A 167, 216 (1938).
- (4) Datta, Chakravarty, PNISI 2, 297 (1941).
- (5) Romand, AP(Paris) (12) 4, 527 (1949).
- (6) Naudé, Verleger, PPS 63, 470 (1950).
- (7) Thompson, Williams, Callomon, SA 5, 315 (1952).
- (8) Hansler, Oetjen, JCP 21, 1340 (1953).
- (9) Schurin, Rollefson, JCP 26, 1089 (1957).
- (10) Watanabe, JCP 26, 542 (1957).
- (11) Mould, Price, Wilkinson, SA 16, 479 (1960).
- (12) Plyler, JRNBS A 64, 377 (1960).
- (13) Barrow, Stamper, PRS A 263, 259, 277 (1961).
- (14) Stamper, Barrow, JPC 65, 250 (1961).
- (15) Stamper, CJP 40, 1279 (1962).
- (16) Babrov, JCP 40, 831 (1964).
- (17) Jones, Gordy, PR A 136, 1229 (1964).
- (18) Babrov, Shabott, Rao, JCP 42, 4124 (1965).
- (19) Chamberlain, Gebbie, Nature 208, 480 (1965).
- (20) James, Thibault, JCP 42, 1450 (1965).
- (21) Rank, Fink, Wiggins, JMS 18, 170 (1965).
- (22) Atwood, Vu, Vodar, SA A 23, 553 (1967).
- (23) Frost, McDowell, Vroom, JCP 46, 4255 (1967).
- (24) Jacobi, JMS 22, 76 (1967).
- (25) Pourcin, Bachet, Coulon, CR B 264, 975 (1967).
- (26) Tokuhiko, JCP 47, 109 (1967).
- (27) Weiss, Cole, JCP 46, 644 (1967).
- (28) Huebert, Martin, JPC 72, 3046 (1968).
- (29) Lempka, Passmore, Price, PRS A 304, 53 (1968).
- (30) Rao, Lindquist, CJP 46, 2739 (1968).
- (31) Van Dijk, Dymanus, CPL 4, 170 (1969).
- (32) Ginter, Tilford, JMS 34, 206 (1970).
- (33) Gustafson, Rao, CJP 48, 330 (1970).
- (34) Tipping, Herman, JMS 36, 404 (1970).
- (35) Van Dijk, Dymanus, CPL 5, 387 (1970).
- (36) Ginter, Tilford, JMS 37, 159 (1971).
- (37) Rao, JP B 4, 791 (1971).
- (38) Bunker, JMS 42, 478 (1972).
- (39) Delwiche, Natalis, Momigny, Collin, JESRP 1, 219 (1972).
- (40) Urquhart, Clark, Rao, ZN 27 a, 1563 (1972).
- (41) Bernage, Niay, Bocquet, Houdart, RPA 8, 333 (1973);
CR B 278, 235 (1974).
- (42) Dabbousi, Meerts, de Leeuw, Dymanus, CP 2, 473 (1973).
- (43) Terwilliger, Smith, JMS 50, 30 (1974).
- (44) Van Dijk, Dymanus, CP 6, 474 (1974).
- (45) Cherlow, Hyatt, Porto, JCP 63, 3996 (1975).
- (46) Terwilliger, Smith, JCP 63, 1008 (1975).
- (47) Ogilvie, Koo, JMS 61, 332 (1976).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^2\text{H}^81\text{Br}$		$\mu = 1.96518641$ $D_0^0 = 3.804 \text{ eV}^a$ I.P. = 11.67_3 eV^b Numerous absorption bands above 114000 cm^{-1} ; see ^1HBr .								DEC 1976 A
M ($^1\Sigma^+$) (109374)		[1000]	$v=0\dots 5$ observed. } See ^1HBr .					M \leftarrow X,	108937	(13)*
L ($^1\Sigma^+, ^1\Pi$) (104141)		[971]	$v=0\dots 4$ observed. }					L \leftarrow X,	(103690)	(13)*
		Further absorption bands of doubtful assignment between 72000 and 83800 cm^{-1} .								(6)
K ^c 1 (83908)		(1792) ^d		[4.121] ^e		[0.80]	[1.442 ₈]	K \leftarrow X, R	83867.1 ^f Z	(6)
J ^c 1 (81248)		(1781) ^d		[4.083] ^g		[1.36]	[1.449 ₅]	J \leftarrow X, R	81202.2 ^f Z	(6)*
I ^c 1 (80442)		(1797) ^d		[4.107]		[1.38]	[1.445 ₂]	I \leftarrow X, R	80403.8 ^f Z	(6)
g ($^3\Sigma^-$) ⁰⁺ (78125)		[1440.6]	Z	[3.79]	(0.40) ^h	[14]	[1.50 ₄]	g \leftarrow X, R	77908.8 Z	(6)(10)
F $^1\Delta$ [77989.0]				[4.095]			[1.447 ₃]	F \leftarrow X, R	77052.3 Z	(6)(10)
f ₁ $^3\Delta_1$ (76787)		[1657.3]	Z	4.06 ₄	0.07 ₆		1.453	f ₁ \leftarrow X, R	76679.2 Z	(6)(10)
D $^1\Pi$ (76280)		[1732.6]	Z	4.128 ⁱ	0.076		1.441 ₅	D \leftarrow X, R	76209.1 Z	(6)(10)*
d ₀ $^3\Pi_0$ [77027.4]				[3.99 ₃] ^j			[1.466]	d ₀ \leftarrow X, R	76090.7 Z	(10)*
E ($^1\Sigma^+$) ⁰⁺ (75682)		[1365]	Z	[3.953]	(0.78) ^h		[1.472 ₉]	E \leftarrow X, R	75428.1 Z	(6)(10)
V $^1\Sigma^+$		Extensive absorption system above 75700 cm^{-1} , incompletely analysed because of strong perturbations. B_v values range from 1.68 to 2.12.						V \leftarrow X, R		(10)
f ₂ $^3\Delta_2$ (74370)		[1660.3]	Z	4.29 ₄	0.097	[2.4]	1.413	f ₂ \leftarrow X, R	74263.1 Z	(6)(10)*
f ₃ $^3\Delta_3$ [75088.6]		Weak transition.		[3.83]		[-2.1]	[1.49 ₇]	f ₃ \leftarrow X, R	74151.9 Z	(10)*
e $^3\Sigma^+$ [74677]		Very diffuse, unresolved band.						e \leftarrow X,	73740	(10)
d ₁ $^3\Pi_1$ [74499]		Diffuse band, rotational structure unresolved.						d ₁ \leftarrow X, R	73562	(6)(10)
d ₂ $^3\Pi_2$ [74391.5]				[3.906] ^k		[0.36]	[1.482]	d ₂ \leftarrow X, R	73454.8 Z	(6)(10)*
C $^1\Pi$ 70563		1811.2	Z 25.5	4.02 ^l	0.10 ₅		1.46 ₁	C \leftarrow X, R	(70501) H ^q	(6)(8)*

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^2\text{H}^{81}\text{Br}$ (continued)										
$b_0 \quad ^3\Pi_0 \quad \begin{matrix} 0^+ \\ 0^- \end{matrix}$	$\begin{matrix} [69837.1] \\ [69832] \end{matrix}$				$[4.08_2]^m$		$[1.450]$	$b_0 \leftarrow X, \quad \begin{matrix} R \quad 68900.4 \quad Z \\ R \quad (68895) \end{matrix}$	$(6)^* (8)^*$	
$b_1 \quad ^3\Pi_1$	67113.9	1814	$Z \quad 27$	4.10^n	0.09		1.44_6	$b_1 \leftarrow X, \quad R \quad 67077.5 \quad Z$	$(6)(8)$	
$b_2 \quad ^3\Pi_2$	$[67290.7]$				$[4.01_8]^m$		$[1.461]$	$b_2 \leftarrow X, \quad R \quad 66354.0 \quad Z$	$(6)(8)$	
$A \quad (^1\Pi)$		Continuous absorption beginning at $\sim 39000 \text{ cm}^{-1}$.						$A \leftarrow X,$	(1)	
$X \quad ^1\Sigma^+$	0	1884.75	$Z \quad 22.71_8^o$	$[4.245596]^p$	0.083_8	$[0.8832]^p$	1.4145	Rot.-vibr. sp.^q $\text{Rotation spectrum}^r$	$(2)(5)$ $(3)(4)(9)(12)$	

^2HBr : a From $D_0(^1\text{HBr})$.

b From the photoelectron sp. (11) of the isotopic mixture.

c See d of ^1HBr .

d See e of ^1HBr .

e Ω -type doubling, $\Delta v_{ef} \approx + 0.0371 J(J+1)$.

f Bands {35}, {27}, {26} of (6).

g Ω -type doubling, $\Delta v_{ef} = + 0.0314 J(J+1)$.

h $v=0$ and 1 only; $v=1$ is perturbed.

i From P, R branches. $B_0(Q) = 4.109$.

j From P, R branches. $B_0(Q) = 3.92_6$.

k Branches are slightly diffuse.

l Diffuse rotational structure; $v=0\dots 4$.

m Slightly diffuse lines.

n $v=2, 3$ diffuse. Slightly diffuse lines for $v=0, 1$.

o $w_e y_e = - 0.010_6$.

p Microwave value (9)(12).

q 1-0, 2-0, 3-0 bands in absorption (2), $\Delta v=1$ sequence in

emission (5).

$r_{\mu_{el}}(v=0) = 0.8233 \text{ D}$ from Stark effect of 1-0 line (12).

Quadrupole and other hyperfine coupling const. (7)(9)(12).

(1) See ref. (1) of ^1HBr .

(2) Keller, Nielsen, JCP 22, 294 (1954).

(3) Palik, JCP 23, 217 (1955).

(4) Cowan, Gordy, PR 111, 209 (1958)

(5) See ref. (11) of ^1HBr .

(6) See ref. (15) of ^1HBr .

(7) See ref. (26) of ^1HBr .

(8) See ref. (32) of ^1HBr .

(9) De Lucia, Helminger, Gordy, PR A 3, 1849 (1971).

(10) See ref. (36) of ^1HBr .

(11) See ref. (39) of ^1HBr .

(12) See ref. (44) of ^1HBr .

(13) See ref. (43) of ^1HBr .

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^3\text{H}^{81}\text{Br}$ X $1\Sigma^+$ 0		$\mu = 2.9076700_9$ [1519.26] ^b Z (15.4 ₈)	$D_0^0 = 3.825 \text{ eV}^a$ [2.874466] ^c	0.0459 ^b	0.45 ^b	1.4145 ₆		Rotation-vibration b. Rotation sp. ^d		DEC 1976 A (2) (1)
$^1\text{HBr}^+$ A $2\Sigma^+$ 28421.0 X $2\Pi_i$ 0 ^h		1404.0 ^b 37.7 ₅ ^b 2441.5 ₂ ⁱ Z 47.4 ₀ ^j	$D_0^0 = 3.894 \text{ eV}^a$ 5.970 ₂ ^{cd} 8.072 ₁ ^k	0.247 ₆ 0.236 ₃	4.30 ₀ ^e [3.48]	1.6842 1.4484		A \rightarrow X, ^f R 27904.6 ^g Z		DEC 1976 A (1)(2)(3) (6)*
$^2\text{HBr}^+$ A $2\Sigma^+$ 28421.2 X $2\Pi_i$ 0 ^o		999.2 ₅ Z 19.1 ₂ 1734.3 ₆ ⁱ Z 22.1 ₈ ^p	$D_0^0 = 3.937 \text{ eV}^l$ 3.024 ₁ ^{mn} 4.087 ₇ ^q	0.089 ₄ 0.084 ₈	1.1 ₀ 0.87 ₀	1.6842 1.4486		A \rightarrow X, R 28054.4 ^g Z		DEC 1976 A (3)(6)
$^1\text{HBr}^-$		Resonances due to inverse preionization have been found in the transmission of electrons through HBr in the energy range 8.0 - 10.8 and 11.5 - 13.2 eV. They correspond to excited states of HBr^- in which two electrons are in Rydberg orbitals $(ns\sigma)^2$, $ns\sigma np\sigma$, $(np\sigma)^2$, ... while the core is in the X $2\Pi_{3/2}$ or A $2\Sigma^+$ state of HBr^+ .								DEC 1976 (1)

³HBr: ^aFrom $D_0^0(^1\text{HBr})$.

^bFrom the rotation-vibration spectrum of the isotopic mixture (⁷⁹,⁸¹Br).

^cFrom the microwave spectrum (1) assuming the infrared D value.

^dQuadrupole coupling constants (3).

(1) Burrus, Gordy, Benjamin, Livingston, PR 27, 1661 (1955).

(2) Jones, Robinson, JCP 24, 1246 (1956).

(3) Tokuhira, JCP 47, 109 (1967).

¹HBr⁺, ²HBr⁺:

^aFrom the predissociation in the A $2\Sigma^+$ state (4); see ^d. $D_0^0(^1\text{HBr}) + \text{I.P.}(\text{Br}) - \text{I.P.}(^1\text{HBr}) = 3.90_2 \text{ eV}$.

^bFrom isotope relations and the constants for DBr⁺ (6). (2) derive $\Delta G(\frac{1}{2}) = 1328.7$ from band origins.

^cSpin splitting constant $\gamma(v=0) = 2.10_5$; small variation with N.

^dOnly $v'=0$ and 1 observed in emission. (4) have observed a sharp breaking-off at $N'=12$ for $v'=1$ and a less distinct breaking-off at $N'=21$ for $v'=0$ yielding a dissociation limit at $31407 \pm 20 \text{ cm}^{-1}$. In the photoelectron spectrum of HBr (5) the bands with $v'=2$ and 3 are as narrow as those with $v'=0$ and 1 but bands with $v' \geq 4$ are strongly broadened indicating strong predissociation (lifetime $\sim 2 \times 10^{-14} \text{ s}$).

^e $\beta_e = -0.01_4 \times 10^{-4}$.

^fTransition moment variation with r from observed vibrational intensity distribution and calculated Franck-Condon factors (7).

¹HBr⁺, ²HBr⁺ (continued):

^eReferring in the lower state to the zero point of the Hill-Van Vleck formula.

^h $A_v = -2652.8_0 + 2.81(v+\frac{1}{2})$.

ⁱValue for the heavier isotope (⁸¹Br).

^j $w_e v_e = +0.40$.

^k Λ -type doubling constants ($p \approx 2.05$) in (2)(6).

^lFrom $D_0^0(^1\text{HBr}^+)$.

^mSpin splitting constant $\gamma(v=0) = 1.06_8$.

ⁿOnly $v'=0,1,2$ observed in emission; breaking-off for $N' > 12$ of $v'=2$ (4). In the photoelectron spectrum $v' = 0 \dots 8$ have been observed (5) but the bands with $v'=6,7,8$ are very broad indicating strong predissociation beginning at the same energy as in ¹HBr⁺.

^o $A_0 = -2651.4_5$, $A_1 = -2649.5_4$, ...

^p $w_e v_e = -0.1$.

^q Λ -type doubling constants ($p \approx 1.05$) in (6).

(1) Norling, ZP 25, 179 (1935).

(2) Barrow, Caunt, PPS 66, 617 (1953).

(3) Marsigny, Lebreton, Ferran, Lagrange, CR C 266, 176, 1731 (1968); Marsigny, Lebreton, Petit, CR C 270, 1632 (1970).

(4) Haugh, Bayes, JPC 75, 1472 (1971).

(5) Delwiche, Natalis, Momigny, Collin, JESRP 1, 219 (1973).

(6) Lebreton, JCPPB 70, 1188 (1973).

(7) Haugh, Schneider, Smith, JMS 51, 123 (1974).

¹HBr⁻: (1) Spence, Noguchi, JCP 63, 505 (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
H^{35}Cl		$\mu = 0.97959272$ $D_0^0 = 4.433_6 \text{ eV}^a$ I.P. = 12.74_8 eV^b Rydberg series corresponding to excitation of a 2p electron. Numerous absorption bands above 123000 cm^{-1} , tentatively assigned to higher members of the Rydberg series starting with L and M and converging to A $^2\Sigma^+$ of HCl^+ .						200-210 eV		DEC 1976 A (50)(60)	
M ($^1\Sigma^+$)	(117811)	[1529] $\nu=0\dots 5$ observed. Assigned as $3p6\ 3p\pi^4\ 5s6^{\cdot c}$						M \leftarrow X,	117093	(55)*	
L ($^1\Sigma^+, ^1\Pi$)	111280	1531 52 Assigned as $3p6\ 3p\pi^4\ 4p6^{\cdot c}/\pi^{\cdot c}$						L \leftarrow X,	110555	(55)*	
		Many other absorption bands in the region $83000 - 93000 \text{ cm}^{-1}$ corresponding to Rydberg states strongly perturbed by the V $^1\Sigma^+$ state which itself gives rise to many perturbed bands.								(62)	
K $^1\Pi$	(89861)	[2604.6]	Z	[9.230] ^d		[-12.6] ^d	[1.3654]	K \leftarrow X,	R 89680.5	Z (62)	
H $^1\Sigma^+$	(89120)	[2093.8]	Z	[8.4410]		[8.93]	[1.4278]	H \leftarrow X,	R 88684.5	Z (62)	
E $^1\Sigma^+$	(84193)	[2138.6]	Z	[6.6423]		[36.2]	[1.6096]	E \leftarrow X,	R 83780.2	Z (62)	
g ($^3\Sigma^-$) ₁	^e [84329.7]			[10.36] ^f		[17] ^f	[1.28 ₉]	g \leftarrow X,	82847.4	Z (48)*	
f ₁ $^3\Delta_1$	^e [84006.1]			[10.27 ₀] ^g		[-13] ^g	[1.294]	f ₁ \leftarrow X,	82523.8	Z (48)*	
D $^1\Pi$	^h [83972.0]			[9.79 ₄] ⁱ		[20.5] ⁱ	[1.326]	D \leftarrow X,	R 82489.7	Z (48)*	
d ₀ $^3\Pi_0$	^h [83753.6]			[9.40 ₄] ^j		[-2.2] ^j	[1.353]	d ₀ \leftarrow X,	R 82271.3	Z (48)*	
f ₂ $^3\Delta_2$	^e [83497.7]			[10.85 ₁] ^k		[29.5] ^k	[1.259]	f ₂ \leftarrow X,	V 82015.4	Z (48)*	
f ₃ $^3\Delta_3$	^e [83308.2]			[9.45] ^g		[-1.3] ^g	[1.34 ₉]	f ₃ \leftarrow X,	R 81825.9	Z (48)*	
d ₁ $^3\Pi_1$	^h [83255.6]			[9.76 ₈] ^l		[8] ^l	[1.327]	d ₁ \leftarrow X,	R 81773.3	Z (48)*	
d ₂ $^3\Pi_2$	^h [83083.0]			[8.63 ₂] ^m		[-14] ^m	[1.412]	d ₂ \leftarrow X,	R 81600.7	Z (48)*	
C $^1\Pi$	ⁿ 77575	[2684.0]	Z	^o [9.33 ₃]	^o		[1.358]	C \leftarrow X, ^p	R 77485.3	Z (1)* (44)	
V $^1\Sigma^+$	^q 77293.0	877.16	Z	16.04 ^r	2.727	-0.026	1.02 ^r	2.512	V \leftrightarrow X, ^s	R 76245.3	Z (8)(9)(48)*
		Continuous emission spectrum with maximum at 38900 cm^{-1} .						V \rightarrow A		(9)	

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^1\text{H}^{35}\text{Cl}$ (continued)										
$b_0 \ ^3\Pi_0$	n (75617)	[2712]		[10.36] ^t			[1.289]	$b_0 \leftarrow X, ^u$	75490.4 Z	(1)(44)*
$b_1 \ ^3\Pi_1$	n (75195)	(2900)	(79)	[9.87] ^t			[1.320]	$b_1 \leftarrow X, R$	75142.6 Z	(1)(44)*
$b_2 \ ^3\Pi_2$	n [76322.2]			[9.18] ^t			[1.369]	$b_2 \leftarrow X, ^u R$	74839.9 Z	(1)(44)*
$A \ (^1\Pi)$	v	Continuous absorption starting at 44000 cm^{-1} , maximum ^w at 65500 cm^{-1}						$A \leftarrow X$		(2)(3)

$^1\text{H}^{35}\text{Cl}$: ^aFrom $D_0^0(\text{H}_2)$, $D_0^0(\text{Cl}_2)$, and $\Delta H_{f0}^0(\text{HCl})$.

^bFrom the photoelectron spectrum (33)(38)(46); photo-ionization measurements give similar results (20)(27). A somewhat smaller I.P.(12.73₀ eV) may be derived from the second band system in the photoelectron spectrum at 16.25₄ eV corresponding to $A \ ^2\Sigma^+$ of HCl^+ . Higher ionization potentials at 207.1 and 208.7 eV correspond to the removal of a 2p electron (50).

^cStrongly broadened by preionization (lifetime $1.1 \times 10^{-14} \text{ s}$)(55).

^dAverage B, D values; $B(R,P) - B(Q) = + 0.385$.

^eConfiguration $\dots 6^2 \pi^3 4p\pi$.

^fAverage B, D values; $B(1^+) - B(1^-) = - 0.06_0$.

^gRefers to Δ^+ ; Q branch not resolved.

^hConfiguration $\dots 6^2 \pi^3 4p6$.

ⁱAverage B, D values; $B(\Pi^+) - B(\Pi^-) = + 0.063$.

^jAverage B, D values; $B(\Pi^+) - B(\Pi^-) = - 0.04_0$.

^kAverage B, D values; $B(\Delta^+) - B(\Delta^-) = - 0.03_0$.

^lAverage B, D values; $B(\Pi^+) - B(\Pi^-) = - 0.16_0$.

^mAverage B, D values; $B(\Pi^+) - B(\Pi^-) = - 0.06_7$.

ⁿConfiguration $\dots 6^2 \pi^3 4s6$.

^o $v=1,2,3$ are increasingly diffuse; $B_1 = 9.29_6$. (44) give

$\omega_e = 2817.5$, $\omega_e x_e = 66.0$, $B_e = 9.44$, $\alpha_e = 0.15$.

^pAlso observed in inert matrices (57).

^qTypical "V" state with configuration $\dots 6^4 \pi^4 6^*$.

^r $\omega_e y_e = 0.113_3$; $\beta_e = 0.2_0 \times 10^{-4}$.

^sVery extended progression in absorption, not yet analyzed in detail. The higher vibrational levels are strongly perturbed by Rydberg states (48)(62). The vibrational and rotational constants given were obtained from the emission spectrum with $v \leq 3$ (8)(9) but because of the perturbations have only very limited meaning.

^tDiffuse rotational structure; 1-0 and 2-0 are increasingly diffuse.

^uThe $b_2 \leftarrow X$ and $b_0 \leftarrow X$ components have only 1/50 of the intensity of $b_1 \leftarrow X$.

^vConfiguration $\dots 6^2 \pi^3 6^*$.

^wAbsorption coefficient $k=40$.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^1\text{H}^{35}\text{Cl}$ (continued)										
X $1\Sigma^+$	0	2990.946 ₃ ^x	52.8186 ^y	10.59341 ₆ ^{xz}	0.30718 ₁ ^{a'}	5.3194 ^{zb'}	1.27455 ₂ ^{c'}	Rot.-vibr. bands ^{d'e'} Rotation spectrum ^{f'e'} Raman cross sections Mol. beam electric ^{g'} and magnetic ^{h'} reson.	(19)(28) (4)(23)(52) (58) (41)(64) (37)	

$^1\text{H}^{35}\text{Cl}$ (continued):

^xApplying the Dunham corrections (28) obtain $\omega_e = 2991.0904$ and $B_e = 10.593553$. Additional corrections (adiabatic, non-adiabatic) discussed by (49). Vibrational levels up to $v=5$ have been observed in infrared absorption (12)(19)(28) and emission (10), higher levels in the $V \rightarrow X$ bands (8)(9). Dunham potential coefficients (61). Most recent ab initio values of the ground state molecular constants (59); charge distribution (40).

^y $\omega_e y_e = + 0.22437$, $\omega_e z_e = - 0.01218$ (28).

^zSlightly different constants in (11)(26)(31). These papers and (39) give also constants for H^{37}Cl .

^{a'} $+ 0.0017724(v+\frac{1}{2})^2 - 0.0001201(v+\frac{1}{2})^3$.

^{b'} $- 7.51_0 \times 10^{-6}(v+\frac{1}{2}) + 4.0_0 \times 10^{-7}(v+\frac{1}{2})^2$; higher order terms in (28). See also (30).

^{c'}Uncorrected value from the $B_e (= Y_{01})$ given in the table. The internuclear distance at the minimum of the Born-Oppenheimer curve is $r_e = 1.2746149 \text{ \AA}$ (49)(63).

^{d'}Absolute intensities ($\text{cm}^{-2} \text{ atm}^{-1}$) of the

1-0 band: 130 (5)

2-0 band: 2.9 (5)

3.70 (17)(45)

3-0 band: 0.023 (5)

^{e'}Pressure-induced shifts (by foreign gases) of rotation-vibration and rotation lines (13)(14)(21)(22)(24). For discussions of pressure-induced bands and pure rotation lines ($\Delta J=2$) see (32)(36). Self and foreign-gas line broadening (5)(7)(16)(17)(18)(29)(43)(45)(47)(52). Infrared absorption in liquid and solid phases (42)(51).

^{f'}Absolute intensity measurements (25)(34).

^{g'} $\mu_{el}(v=0,1,2) = 1.1085, 1.1390, 1.1685 \text{ D}$, resp. (41).

Dipole moment function (41)(54); see also (53)(56).

$g_J = 0.4594$, also quadrupole and other hyperfine coupling constants (41)(64); see also (35)(53).

^{h'}Proton spin - rotation interaction constant (15)(37).

- ¹
- HCA: (1) Price, PRS A
- 167
- , 216 (1938).
-
- (2) Datta, Banerjee, PNISI
- 7
- , 305 (1941).
-
- (3) Romand, AP(Paris) (12)
- 4
- , 527 (1949).
-
- (4) Hansler, Oetjen, JCP
- 21
- , 1340 (1953).
-
- (5) Benedict, Herman, Moore, Silverman, CJP
- 34
- , 850 (1956); JCP
- 26
- , 1671 (1957).
-
- (6) Legay, CaP
- 11
- , 383 (1957); RO
- 37
- , 11 (1958).
-
- (7) Babrov, Ameer, Benesch, JMS
- 3
- , 185 (1959).
-
- (8) Jacques, D.Phil. Thesis (Oxford, 1959).
-
- (9) Jacques, Barrow, PPS
- 73
- , 538 (1959).
-
- (10) Mould, Price, Wilkinson, SA
- 16
- , 479 (1960).
-
- (11) Plyler, Tidwell, ZE
- 64
- , 717 (1960).
-
- (12) Rank, Birtley, Eastman, Rao, Wiggins, JOSA
- 50
- , 1275 (1960).
-
- (13) Rank, Eastman, Birtley, Wiggins, JCP
- 33
- , 323 (1960).
-
- (14) Ben-Reuven, Kimel, Hirshfeld, Jaffe, JCP
- 35
- , 955 (1961).
-
- (15) Leavitt, Baker, Nelson, Ramsey, PR
- 124
- , 1482 (1961).
-
- (16) Goldring, Benesch, CJP
- 40
- , 1801 (1962).
-
- (17) Jaffe, Kimel, Hirshfeld, CJP
- 40
- , 113 (1962).
-
- (18) Plyler, Thibault, JRNS A
- 66
- , 435 (1962).
-
- (19) Rank, Eastman, Rao, Wiggins, JOSA
- 52
- , 1 (1962).
-
- (20) Watanabe, Nakayama, Mottl, JQSRT
- 2
- , 369 (1962).
-
- (21) Gebbie, Stone, PPS
- 82
- , 309 (1963).
-
- (22) Jaffe, Friedmann, Hirshfeld, Ben-Reuven, JCP
- 39
- , 1447
-
- (23) Jones, Gordy, PR A
- 135
- , 295;
- 136
- , 1229 (1964). | (1963).
-
- (24) Jaffe, Hirshfeld, Ben-Reuven, JCP
- 40
- , 1705 (1964).
-
- (25) Chamberlain, Gebbie, Nature
- 208
- , 480 (1965).
-
- (26) Lévy, Rossi, Joffrin, Thanh, JCPPB
- 62
- , 600 (1965).
-
- (27) Nicholson, JCP
- 43
- , 1171 (1965).
-
- (28) Rank, Rao, Wiggins, JMS
- 17
- , 122 (1965).
-
- (29) Alamichel, Legay, JP(Paris)
- 27
- , 233 (1966).
-
- (30) Herman, Asgharian, JCP
- 45
- , 2433 (1966).
-
- (31) Lévy, Rossi, Haeusler, JP(Paris)
- 27
- , 526 (1966).
-
- (32) Atwood, Vu, Vodar, SA A
- 23
- , 553 (1967).
-
- (33) Frost, McDowell, Vroom, JCP
- 46
- , 4255 (1967).
-
- (34) Sanderson, AO
- 6
- , 1527 (1967).
-
- (35) Tokuhiko, JCP
- 47
- , 109 (1967).
-
- (36) Weiss, Cole, JCP
- 46
- , 644 (1967).
-
- (37) Code, Khosla, Ozier, Ramsey, Yi, JCP
- 49
- , 1895 (1968).
-
- (38) Lempka, Passmore, Price, PRS A
- 304
- , 53 (1968).
-
- (39) Webb, Rao, JMS
- 28
- , 121 (1968).
-
- (40) Cade, Bader, Henneker, Keaveny, JCP
- 50
- , 5313 (1969).
-
- (41) Kaiser, JCP
- 53
- , 1686 (1970).
-
- (42) Katz, Ron, CPL
- 7
- , 357 (1970).
-
- (43) Lévy, Mariel-Piollet, Bouanich, Haeusler, JQSRT
- 10
- , 203 (1970).
-
- (44) Tilford, Ginter, Vanderslice, JMS
- 33
- , 505 (1970).
-
- (45) Toth, Hunt, Plyler, JMS
- 35
- , 110 (1970).
-
- (46) Weiss, Lawrence, Young, JCP
- 52
- , 2867 (1970).
-
- (47) Rich, Welsh, CPL
- 11
- , 292 (1971).
-
- (48) Tilford, Ginter, JMS
- 40
- , 568 (1971).
-
- (49) Bunker, JMS
- 42
- , 478 (1972).
-
- (50) Hayes, Brown, PR A
- 6
- , 21 (1972).
-
- (51) Khatibi, Vu, JCPPB
- 69
- , 654, 662, 674 (1972).
-
- (52) Rosenberg, Lightman, Ben-Reuven, JQSRT
- 12
- , 219 (1972).
-
- (53) Bunker, JMS
- 45
- , 151 (1973).
-
- (54) Smith, JQSRT
- 13
- , 717 (1973).
-
- (55) Terwilliger, Smith, JMS
- 45
- , 366 (1973); JCP
- 63
- , 1008 (1975).
-
- (56) Kaiser, JQSRT
- 14
- , 317 (1974).
-
- (57) Boursey, JCP
- 62
- , 3353 (1975).
-
- (58) Cherlow, Hyatt, Porto, JCP
- 63
- , 3996 (1975).
-
- (59) Meyer, Rosmus, JCP
- 63
- , 2356 (1975).
-
- (60) Schwarz, CP
- 11
- , 217 (1975).
-
- (61) Ogilvie, Koo, JMS
- 61
- , 332 (1976).
-
- (62) Douglas, Greening, unpublished.
-
- (63) Watson, JMS
- 45
- , 99 (1973).
-
- (64) de Leeuw, Dymanus, JMS
- 48
- , 427 (1973).

^2HCl : ^aFrom $D_0(^1\text{HCl})$.
^bFrom the photoelectron spectrum (19); via the $A\ ^2\Sigma^+$ state of DCl^+ one finds 12.73_2 eV.
^cAverage B value; $B(R,P) - B(Q) = + 0.1028$.
^dAverage B, D values; $B(\Pi^+) - B(\Pi^-) = + 0.022$ in $v=0$ and $- 0.006$ in $v=1$.
^eAverage B, D values; $B(\Pi^+) - B(\Pi^-) = - 0.022$.
^fAverage B, D values; $B(\Pi^+) - B(\Pi^-) = - 0.05_4$.
^g $\omega_e y_e = + 0.39$.
^h $B_0(\Pi^+) - B_0(\Pi^-) = + 0.0034$ (9). Lines are slightly diffuse but much sharper than in the corresponding ^1HCl bands.
ⁱ $B(\Pi^+) - B(\Pi^-) = + 0.01_0$ (9).
^j $v=1$ and 2 are increasingly diffuse.
^k $\omega_e y_e = + 0.08649$, $\omega_e z_e = - 0.00355$, $\gamma_e = + 0.0004589$, $\delta_e(Y_{31}) = - 0.00002103$ from ^1HCl by isotope relations (8). Constants for $^2\text{H}^{37}\text{Cl}$ in (2)(3)(5)(7)(15).
^lThe rotational constants, derived from infrared data (8), agree with the more recent microwave data of (21).
^m $\beta_e = - 0.013_3 \times 10^{-4}$; $H_e = 2.3_1 \times 10^{-9}$ (7).
ⁿ $1-0, 2-0, 3-0$ bands in absorption (2)(3)(8), $\Delta v=1$ sequence in emission (7); P(7), P(8), P(9) lines of the $2-1$ band observed in $\text{D}_2\text{-Cl}_2$ explosion laser (14). IR absorption in solid argon and other low-temperature matrices, hindered rotation (20).
^oAbsolute intensities [$\text{cm}^{-2}\text{atm}^{-1}$] of the

1-0 band:	66.6	(4)
2-0 band:	1.06	(4)
3-0 band:	0.0059	(4)

^pPressure broadening in the $1-0$ band (both self-broadening and broadening by foreign gases) (10)(12), in the rotation spectrum (23); pressure shifts (11).

$q_{el}(v=0) = 1.1033$ D, $q_{el}(v=1) = 1.1256$ D (16). Dipole moment function (16)(24); see also (26). Quadrupole and other hyperfine coupling constants (16); see also (13).

- (1) See ref. (4) of ^1HCl .
- (2) Pickworth, Thompson, PRS A 218, 37 (1953).
- (3) Van Horne, Hause, JCP 25, 56 (1956).
- (4) See ref. (5) of ^1HCl .
- (5) Cowan, Gordy, PR 111, 209 (1958).
- (6) Burrus, JCP 31, 1270 (1959).
- (7) See ref. (10) of ^1HCl .
- (8) See ref. (19) of ^1HCl .
- (9) Stamper, CJP 40, 1274 (1962).
- (10) Crane-Robinson, Thompson, PRS A 272, 441, 453 (1963).
- (11) See ref. (24) of ^1HCl .
- (12) James, Thibault, JCP 40, 534 (1964).
- (13) See ref. (35) of ^1HCl .
- (14) Corneil, Pimentel, JCP 42, 1379 (1968).
- (15) See ref. (39) of ^1HCl .
- (16) See ref. (41) of ^1HCl .
- (17) See ref. (42) of ^1HCl .
- (18) See ref. (44) of ^1HCl .
- (19) See ref. (46) of ^1HCl .
- (20) Davies, Hallam, TFS 67, 3176 (1971).
- (21) De Lucia, Helminger, Gordy, PR A 3, 1849 (1971).
- (22) See ref. (48) of ^1HCl .
- (23) See ref. (52) of ^1HCl .
- (24) See ref. (54) of ^1HCl .
- (25) See ref. (55) of ^1HCl .
- (26) See ref. (56) of ^1HCl .
- (27) See ref. (62) of ^1HCl .

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^3\text{H}^{35}\text{Cl}$ X $1\Sigma^+$ 0		$\mu = 2.7765715_3$ [1739.10] Z (18.64)		$D_0^0 = 4.507_8 \text{ eV}^a$ [3.705089] ^b	0.0611 ^b	0.77 ^b	1.2749	Rotation-vibration sp. Rotation sp. ^c		DEC 1976 (2) (1)
$^1\text{H}^{35}\text{Cl}^+$ A $2\Sigma^+$ 28626.5 X $2\Pi_i$ 0 ^h		1606.4 ₇ ^b Z 40.3 ₁ ^b 2673.69 ⁱ Z 52.537 ⁱ		$D_0^0 = 4.65_3 \text{ eV}^a$ 7.505 ₄ ^{bcd} 0.331 ₃ ^b 9.9566 ₁ ^{jk} 0.3271 ₆ ^j		[6.43 ₅] ^e 1.5142 [5.47 ₇] ^l 1.31468		A \rightarrow X, ^f R 28095.97 ^g Z		DEC 1976 A (1)(3)(5)
$^2\text{H}^{35}\text{Cl}^+$ A $2\Sigma^+$ 28629.2 X $2\Pi_i$ 0 ^p		1152.0 ₉ ^b Z 20.4 ₅ ^b 1918.56 ⁱ Z 27.263 ⁱ		$D_0^0 = 4.69_7 \text{ eV}^m$ 3.859 ₅ ^{bn} 0.122 ₂ ^b 5.1216 ₄ ^{qk} 0.1203 ₇ ^q		[1.717] ^o 1.5144 [1.459] ^r 1.31466		A \rightarrow X, ^f R 28247.65 ^g Z		DEC 1976 (1)(3)(5)
$^1\text{HCl}^-$ X $2\Sigma^+$ a				Resonances due to inverse preionization have been found in the transmission of electrons through HCl in the energy range 9.1 - 11.0 and 12.5 - 13.9 eV. Interpretation analogous to HBr ⁻ .						DEC 1976 A (2)

^3HCl : ^aFrom $D_0(^1\text{HCl})$.

^b B_0 from the microwave spectrum (1), α_e and D_e from the infrared spectrum (2). (1)(2) give also data for $T^{37}\text{Cl}$.

^cNuclear quadrupole coupling constants (3).

(1) Burrus, Gordy, Benjamin, Livingston, PR 97, 1661 (1955).

(2) Jones, Robinson, JCP 24, 1246 (1956).

(3) Tokuhito, JCP 47, 109 (1967).

$^1\text{HCl}^+$, $^2\text{HCl}^+$:

^aRefers to $^2\Pi_{3/2}$; from $D_0(^1\text{HCl}) + \text{I.P.}(\text{Cl}) - \text{I.P.}(\text{HCl})$.

^bEquilibrium values of (3); $G(v)$ and B_v are far from linear but higher terms in $(v+\frac{1}{2})$ have not been given.

(3)(5) give T_v , B_v values up to $v=6$ (HCl^+) and 9 (DCl^+); their T_v values differ systematically by $\sim 2.34 \text{ cm}^{-1}$.

^cSpin doubling constants for $v=0\dots 6$ in (3)(5);

$f(v=0; N) = + 0.5942 - 0.000034 N(N+1)$.

^dHigher vibrational levels are predicted (2) to be pre-dissociated by the $^4\Pi$ state from $\text{H}(^2\text{S}) + \text{Cl}^+(^3\text{P})$.

^e $H_0 = 2.30 \times 10^{-8}$. Additional D_v , H_v values in (3)(5).

^fVariation of transition moment with r derived from observed intensities by (4) who also give Franck-Condon factors.

^gFrom (5); (3) give 28098.35 (HCl^+) and 28250.08 (DCl^+); see ^b.

^hSpin-orbit coupling constants for $v=0,1,2$ in (5);

$A(v=0; J) = - 648.13_1 + 0.00209(J+\frac{1}{2})^2$.

ⁱFrom $\Delta G(1/2)$ and $\Delta G(3/2)$ of (5).

^jFrom B_0 , B_1 , B_2 of (5); $f_e = + 0.0026_6$.

^k Λ -type doubl. const. [$p \approx 0.60(\text{HCl}^+)$, $0.31(\text{DCl}^+)$] in (5).

^l $H_0 = 1.52 \times 10^{-8}$; additional D_v , H_v values in (5).

$^1\text{HCl}^+$, $^2\text{HCl}^+$ (continued):

^mRefers to $^2\Pi_{3/2}$; from $D_0(\text{DCl}) + \text{I.P.}(\text{Cl}) - \text{I.P.}(\text{DCl})$.

ⁿSpin-doubling constants for $v=0\dots 9$ in (3)(5);

$f(v=0; N) = + 0.3060 - 8.6 \times 10^{-6} N(N+1)$.

^o $H_0 = 0.40 \times 10^{-8}$; additional D_v , H_v values in (3)(5).

^pSpin-orbit coupling constants for $v=0,1,2$ in (5);

$A(v=0; J) = - 648.17_0 + 0.00095(J+\frac{1}{2})^2$.

^qFrom B_0 , B_1 , B_2 of (5); $f_e = + 0.00061$.

^r $H_0 = + 0.29 \times 10^{-8}$; additional D_v , H_v values in (5).

(1) Norling, ZP 104, 638; 106, 177 (1937).

(2) Raftery, Richards, JP B 6, 1301 (1973).

(3) Sheasley, Mathews, JMS 47, 420 (1973).

(4) Haugh, Schneider, Smith, JMS 51, 123 (1974).

(5) Saenger, Zare, Mathews, JMS 61, 216 (1976).

$^1\text{HCl}^-$: ^aThe ground state $X \ ^2\Sigma^+$ of HCl^- lies presumably above the ground state $X \ ^1\Sigma^+$ of HCl ; see (1).

(1) Fiquet-Fayard, JP B 7, 810 (1974).

(2) Spence, Noguchi, JCP 62, 505 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^4\text{He}_2$		$\mu = 2.0013016_3$		$D_e^0 = 0.00090 \text{ eV}^a$ $D_0(a^3\Sigma_u^+) = 1.850 \text{ eV}^b$ $D_0(A^1\Sigma_u^+) = 2.355 \text{ eV}^b$		I.P. = 22.223 eV^c				NOV 1976 A
				Rydberg series of $np\pi$ $^3\Pi_g$ levels (b, e, i, l, p, r, s, t, u, ...)				$\nu^d = 34302.20 - R/(n - 0.071)^2$, $n = 2 \dots 17$.		(23)(39)
				Rydberg series of $np\sigma$ $^3\Sigma_g^+$ levels (c, g, k', n, p', r', s', t', ...)				$\nu^d = 34302.20 - R/(n - 0.777)^2$, $n = 3 \dots 12$.		(23)(39)
u $^3\Pi_g$ 10p π 177291		$[1628.6_9]^e$ Z (35.2 ₅)		7.21_2^e	0.22_2^e	$[5.03]^e$	1.081	u \rightarrow a, R	33189.16 Z	(23)
t' $^3\Sigma_g^+$ 10p σ [177969]				$[8.27]^f$				t' \rightarrow a, V	33026.6 Z	(23)
t $^3\Pi_g$ 9p π 177027		$[1629.1_5]^g$ Z (35.2 ₅)		7.21_2^g	0.23_0^g	$[5.07]^g$	1.081	t \rightarrow a, R	32925.96 Z	(23)
s' $^3\Sigma_g^+$ 9p σ [177636]				$[8.04]^f$				s' \rightarrow a, V	32693.2 Z	(23)
s $^3\Pi_g$ 8p π 176658		$[1629.30]^h$ Z (35.2 ₅)		7.21_3^h	0.223_4^h	5.1^h	1.080_6	s \rightarrow a, R	32556.66 Z	(23)
r' $^3\Sigma_g^+$ 8p σ [177154]				$[7.78]^f$				r' \rightarrow a, V	32211.7 Z	(23)
r $^3\Pi_g$ 7p π 176117		$(1700.5_6)^i$ (35.2 ₅)		$[7.104_4]^i$	i	$[5.08]^i$	$[1.0889]$	r \rightarrow d, R	11625.3 Z	(39)
								r \rightarrow a, R	32016.56 Z	(23)
p' $^3\Sigma_g^+$ 7p σ [176421]				$[7.543]^f$				p' \rightarrow a,	31478.6 Z	(23)
q $\left\{ \begin{array}{l} ^3\Delta_u \\ ^3\Pi_u \\ ^3\Sigma_u^+ \end{array} \right.$ 6d δ [176195] 6d π [(176169)] 6d σ [176120]				$[7.092]^j$		$[5.0]^j$	$[1.089_8]$	q \rightarrow c, $\left\{ \begin{array}{l} V \\ R \\ R \end{array} \right.$	$\left\{ \begin{array}{l} 20365 \\ (20330) \\ 20288 \end{array} \right.$	(1)(39)
								q \rightarrow b, $\left\{ \begin{array}{l} V \\ R \\ R \end{array} \right.$	$\left\{ \begin{array}{l} 26483 \\ (26466) \\ 26409 \end{array} \right.$	(1)(39)
p $^3\Pi_g$ 6p π 175281		1701.18 Z 35.35		7.220^k	0.224	5.14	1.080_1	p \rightarrow d, R	10788.68 Z	(39)
								p \rightarrow a, R	31179.93 Z	(23)
o $^3\Sigma_u^+$ 6s σ [176001]				$[7.109]$		$[5.1]$	$[1.088_5]$	o \rightarrow c, V	20168.8 Z	(2)(39)
								o \rightarrow b, R	26290.3 Z	(2)(39)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}_2$ (continued)										
n $3\Sigma_g^+$ 6p6	174389	[1619.52] Z (36.5)		7.475_4^l	0.249 ₀	$[7.2_1]^m$	1.0615	n \rightarrow a,	30283.26 Z	(3)(67)
m $\left\{ \begin{array}{l} 3\Delta_u \\ 3\Pi_u \\ 3\Sigma_u^+ \end{array} \right.$	5d6 [174863]							$\left\{ \begin{array}{l} V (19039) \\ R (18944) \\ R 18899 \end{array} \right.$	(39)	
	5d π [(174778)]									
	5d6 [174730]									
l $3\Pi_g$ 5p π	173884	[1633.9 ₆] ^p Z (35.2 ₅)		7.226^p	0.222 ^p	$[5.12]^p$	1.079 ₇	l \rightarrow d, R 9393.9 Z	(39)	
								l \rightarrow a, R 29785.31 Z	(23)	

He_2 : ^aAverage of two independent values for the well depth obtained from measurements of the total (44) and differential (45)(66) elastic scattering cross sections (0.88₈ and 0.90₅ meV, resp.). Ab initio values range from 0.78 to 1.04 meV (33)(43)(51)(53)(56)(64). Both experiment and theory agree that no bound vibrational level exists in the potential well, i.e. $D_0^0 = 0$; see (27)(63). A somewhat higher D_e value (0.99 meV) was derived (61) from the temperature dependence of the relaxation time in dilute ^3He . For measurements of the short-range potential ($0.49 < r(\text{\AA}) < 1.56$) see (57); the long-range potential is discussed by (28)(29).

^bBased on $D_0^0(\text{He}_2^+)$. From a detailed interpretation of the Hopfield continuum and the 600 \AA absorption and emission bands (49) derives $D_e(A^1\Sigma_u^+) = 2.50 \text{ eV}$.

^cRelative to $\text{He}(^1\text{S}) + \text{He}(^1\text{S})$, i.e. $\text{I.P.}(\text{He}_2) = \text{I.P.}(\text{He}) - D_0^0(\text{He}_2^+)$. The I.P. for the lowest stable state (a $^3\Sigma_u^+$) is 4.25297 eV.

^dGiving the $v=0, N=0$ levels (real or hypothetical) of np6

$^3\Sigma_g^+$ and npπ $^3\Pi_g^-$ relative to 2s6 $^3\Sigma_u^+$, $v=0, N=0$.

^eRefers to Π^- . $B_0(^3\Pi^+) \approx 5.6$, strongly affected by l -uncoupling.

^fEffective value, strongly affected by l -uncoupling.

^gRefers to Π^- . $B_0(^3\Pi^+) = 5.87$, strongly affected by l -uncoupling.

^hRefers to Π^- . $B_0(^3\Pi^+) = 6.13$, strongly affected by l -uncoupling.

ⁱConstants refer to Π^- ; $B_0(^3\Pi^+) = 6.37_5$ affected by l -uncoupling. $v=1$ is perturbed; approximate deperturbed constants for Π^- : $B_1 = 6.88_6$, $\Delta G(\frac{1}{2}) = 1629.7$.

^jStrong l -uncoupling. The rotational constants (1) refer to the average of Π^- and Δ^- .

^kRefers to Π^- . $B_0(^3\Pi^+) = 6.630$ affected by l -uncoupling.

^lSeveral small accidental perturbations.

^m $D_1 = 6.8_2 \times 10^{-4}$, $H_0 = 14.2 \times 10^{-8}$, $H_1 \approx -26 \times 10^{-8}$.

ⁿAverage of Π^- and Δ^- as given by (39).

^oAverage of Σ^+ , Π^+ , Δ^+ as given by (39).

^pRefers to Π^- .

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}_2$ (continued)										
k $^3\Sigma_u^+$ 5s σ (173698)		[1635.3]	Z	7.23 ₂	0.23		1.079	k \rightarrow c, V	18683.5 Z	(39)
								k \rightarrow b, R	24804.8 Z	(39)
k' $^3\Sigma_g^+$ 5p σ 172236		1686.90	Z 38.10	7.379 ^a	0.349 ^b	[5.8]	1.068 ₄	k' \rightarrow a, R	28127.58 Z	(67)
j $\left\{ \begin{array}{l} ^3\Delta_u \\ ^3\Pi_u \end{array} \right.$ 4d δ 171573		1702.2 ₄ ^c	Z 35.0 ₇	7.208 ₈ ^c	0.224 ₈ ^d	5.2 ^c	1.0810	j \rightarrow c, $\left\{ \begin{array}{l} V \\ R \end{array} \right.$	$\left\{ \begin{array}{l} 16583.18^c \\ 16400.69^c \end{array} \right.$ Z	(50)
j $\left\{ \begin{array}{l} ^3\Pi_u \\ ^3\Sigma_u^+ \end{array} \right.$ 4d π 171402		1680.9 ₄ ^c	Z 40.8 ₁	7.186 ₀ ^c	0.229 ₆ ^e	5.4 ^c	1.0827	j \rightarrow b, $\left\{ \begin{array}{l} V \\ R \end{array} \right.$	$\left\{ \begin{array}{l} 22704.5^c \\ 22522.0^c \end{array} \right.$ Z	(50)
		1669.7 ₉ ^f	39.0 ₉	Strongly perturbed by ℓ -uncoupling and by interaction with the h state. ^h						
i $^3\Pi_g$ 4p π 171290		[1637.94] ^g	Z (35.2 ₅)	7.242 ^g	0.223 ^g	[5.1 ₄] ^g	1.078 ₅	i \rightarrow a, R	27193.01 Z	(23)(39)
h $^3\Sigma_u^+$ 4s σ (170884)		[1637.9]	Z	7.26 ₄ ^h	0.23	(5.2 ₄)	1.077	h \rightarrow c, V	15870.7 Z	(2)(39)(50)
								h \rightarrow b, R	21992.2 Z	(2)(39)(50)*
g $^3\Sigma_g^+$ 4p σ 167714		[1589.92]	Z (41)	7.220 ₇	0.247 ₈	[5.38] ⁱ	1.0801	g \rightarrow a, R	23597.00 Z	(67)
f $\left\{ \begin{array}{l} ^3\Delta_u \\ ^3\Pi_u \end{array} \right.$ 3d δ 166303		1706.82	Z 35.10	7.230 ^j	0.227 ^k	[5.26] ^l	1.079 ₄	f \rightarrow c, $\left\{ \begin{array}{l} V \\ R \end{array} \right.$	$\left\{ \begin{array}{l} 11316.06 \\ 10864.53 \end{array} \right.$ Z	(17)
f $\left\{ \begin{array}{l} ^3\Pi_u \\ ^3\Sigma_u^+ \end{array} \right.$ 3d π 165877 ^m		1661.48	Z 44.79	7.136 ^j	0.235 ⁿ	[5.34] ^o	1.086 ₅	f \rightarrow b, $\left\{ \begin{array}{l} V \\ R \end{array} \right.$	$\left\{ \begin{array}{l} 17437.3 \\ 16985.8 \end{array} \right.$ Z	(13)* (13)(39)
		1635.77	Z 44.41	7.071 ^j	0.246 ^p	[5.31] ^q	1.091 ₄			
e $^3\Pi_g$ 3p π 165598		1721.22	Z 34.97 ₀ ^s	7.283 ₈ ^r	0.221 ₅ ^t	5.22	1.0754	e \leftrightarrow a, ^u R	21507.26 Z	(36)
d $^3\Sigma_u^+$ 3s σ 164479		1728.01	Z 36.13 ^v	7.341 ₂	0.224 ₄ ^w	5.32	1.0712	d \rightarrow c, V	9502.7 Z	(13)
								d \rightarrow b, R _V	15623.1 Z	(13)*
c $^3\Sigma_g^+$ 3p σ 155053		1583.85	Z 52.7 ₄ ^x	7.004 ₈	0.310 ₅ ^y	[5.56] ^z	1.0966	c \rightarrow a, R	10889.48 Z	(11)
b $^3\Pi_g$ 2p π 148835		1769.07	Z 35.02 ^{a'}	7.447 ₃ ^{b'}	0.219 ₆ ^{c'}	[5.30] ^{d'}	1.0635	b \rightarrow a, R	4768.2 Z	(5)(14)
a $^3\Sigma_u^+$ 2s σ 144048		1808.5 ₆	Z 38.2 ₁ ^{e'f'}	7.703 ₆ ^{g'}	0.228 ₁ ^{h'}	5.56 ^{i'}	1.0457	(a - X)	144935 ^{j'}	

He₂,
^aSeveral small accidental perturbations.
^b $\gamma_e = + 0.030$.
^cThe vibrational and rotational constants refer to Π^- and Δ^- which are less affected by ℓ -uncoupling.
^d $\gamma_e = - 0.0038$.
^e $\gamma_e = - 0.0046$.
^fConstants refer to $N'=1$.
^gConstants refer to $3\Pi^-$.
^h(50) give average effective constants for the four interacting components $j(3\Delta_u^+, 3\Pi_u^+, 3\Sigma_u^+)$ and $h\ 3\Sigma_u^+$.
ⁱ $H_0 = 2.0 \times 10^{-8}$.
^jThese constants are corrected for ℓ -uncoupling effects.
^k $\gamma_e = - 0.0046$.
^l $D_1 = 5.28 \times 10^{-4}$, $D_2 = 5.50 \times 10^{-4}$, $H_0 = 2.5 \times 10^{-8}$.
^mAb initio calculations of $f\ 3\Pi_u$ and $F\ 1\Pi_u$ (10)(26) yield excellent agreement with the observed constants and confirm the presence of substantial potential maxima; see also (9).
ⁿ $\gamma_e = - 0.0069$.
^o $D_1 = 5.34 \times 10^{-4}$, $D_2 = 5.74 \times 10^{-4}$, $H_0 = 2.9 \times 10^{-8}$.
^p $\gamma_e = - 0.0095$.
^q $D_1 = 5.34 \times 10^{-4}$, $D_2 = 5.45 \times 10^{-4}$, $H_0 = 0.91 \times 10^{-8}$.
^rThe rotational constants refer to Π^- (36); $B(3\Pi^-) - B(3\Pi^+) \approx +0.072$. Slightly different constants were given by (4) who also derived constants for ${}^3\text{He}_2$.
^s $w_e\gamma_e = - 0.038$. See also ^r.
^t $\gamma_e = - 0.00138$.

^uObserved in absorption in a pulsed discharge (19).
^v $w_e\gamma_e = - 0.1267$.
^w $\gamma_e = - 0.00273$.
^x $w_e\gamma_e = - 1.2566$, $w_e z_e = - 0.4875$.
^y $+ 0.1629(v+\frac{1}{2})^2 - 0.0655(v+\frac{1}{2})^3$.
^z $D_1 = 5.76 \times 10^{-4}$, $D_2 = 6.11 \times 10^{-4}$, ...; $H_0 = 1.32 \times 10^{-8}$,
 $H_1 = -0.40 \times 10^{-8}$, $H_2 = -5.3 \times 10^{-8}$,
^a $w_e\gamma_e = - 0.0483$.
^bThe constants refer to $3\Pi^-$ and were derived by (13) from the $d, f \rightarrow b$ bands; $B(3\Pi^-) - B(3\Pi^+) \approx + 0.026$. The triplet splitting is partially resolved in the $d \rightarrow b$ bands (13).
^c $\gamma_e = - 0.00170$.
^d $D_1 = 5.34 \times 10^{-4}$, ...; $H_0 = 2.80 \times 10^{-8}$, $H_1 = 3.60 \times 10^{-8}$, ...
^e $w_e\gamma_e = - 0.38$ (36).
^fThere is good experimental (20)(30) and theoretical (7) (21)(48) evidence for a potential maximum in this state. (20) place the maximum at 0.067 eV above the asymptote; the net dissociation energy is 1.850 eV.
^gFrom molecular beam magnetic resonance experiments (58) (65) have determined the triplet splitting for $N=1$ and 3. The splitting constants (extrapolated to $N=0$) are $\lambda = - 0.03666$, $\gamma = - 0.0000808\text{ cm}^{-1}$. An ab initio calculation (55) gives $\lambda = - 0.04089$.
^h $\gamma_e = - 0.00462$ (36).
ⁱ $\beta_e = + 0.07 \times 10^{-4}$; $H_e \approx 2.7 \times 10^{-8}$ (36).
^jEnergy of a ${}^3\Sigma_u^+, v=0, N=0$ above $\text{He}({}^1S) + \text{He}({}^1S)$, based on $D_0({}^0\text{He}_2^+) = 19073\text{ cm}^{-1}$. See also ^c p. 297.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^4\text{He}_2$ (continued)										
S $1\pi_g$	8p π [177515]			(7.21)	(0.22)		(1.08 ₁)	S \rightarrow A, R	30228.6	Z (39)
R $1\pi_g$	7p π [176983]			(7.22)	(0.22)		(1.08 ₀)	R \rightarrow A, R	29696.4	Z (39)
P $1\pi_g$	6p π [176160]			(7.22)	(0.22)		(1.08 ₀)	P \rightarrow A, R	28873.9	Z (39)
M $\left\{ \begin{array}{l} 1\Delta_u \\ 1\pi_u \\ 1\Sigma_u^+ \end{array} \right.$	5d δ [(174838)]			$[7.09]^a$ $[7.07]^b$			[1.09 ₁]	M \rightarrow B, $\left\{ \begin{array}{l} (24050) \\ (24000) \\ (23960) \end{array} \right.$		(39)
	5d π [(174788)]									
	5d σ [(174748)]									
L $1\pi_g$	5p π [174794]			(7.23)	(0.22 ₂)		(1.07 ₉)	L \rightarrow A, R	27507.8	Z (39)
J $\left\{ \begin{array}{l} 1\Delta_u \\ 1\pi_u \\ 1\Sigma_u^+ \end{array} \right.$	4d δ [172416]			$[7.097]^c$		[5.0]	[1.089 ₄]	J \rightarrow C, $\left\{ \begin{array}{l} V \\ R \end{array} \right.$	14183.90 ^c Z 14058.37 ^c Z 13990.32 ^d Z	(50)
	4d π [172290]			$[7.080]^c$		[5.4]	[1.090 ₈]			
	4d σ [172222] ^d			Strongly perturbed by l -uncoupling and interaction with H $1\Sigma_u^+$ ^e						
I $1\pi_g$	4p π [172266]			(7.24 ₂)	(0.22 ₃)		(1.078)	I \rightarrow A, R	24979.6	Z (39)
H $1\Sigma_u^+$	4s σ [171951]			(7.26) ^e	(0.23)		(1.07 ₇)	H \rightarrow C, V	13719.5	Z (39) (50)
								H \rightarrow B, R	21163.5	Z (39) (50)
F $\left\{ \begin{array}{l} 1\Delta_u \\ 1\pi_u \\ 1\Sigma_u^+ \end{array} \right.$	3d δ 166304	1706.59	Z 35.06	7.230 ^g	0.225 ^h	[5.20] ⁱ	1.079 ₄	F \rightarrow B, $\left\{ \begin{array}{l} V \\ R \end{array} \right.$	16360.9 Z 16008.3 Z 15837.5 Z	(12) (17)
	3d π 165971 ^f	1670.57	Z 40.03	7.156 ^g	0.235	[5.24] ^j	1.084 ₉			
	3d σ (165813)	[1564.25]	Z (40)	7.098 ^g	0.246	[5.21] ^k	1.089 ₄			
E $1\pi_g$	3p π 165911	1721.1 ₉	Z 34.76 ^l	7.270 ₅ ^m	0.215 ₆ ⁿ	5.20	1.076 ₄	E \rightarrow A, R	19476.61	Z (36)
D $1\Sigma_u^+$	3s σ 165085	1746.43	Z 35.54	7.365	0.218 ₀ ^o	5.24 ^p	1.069 ₄	D \rightarrow B, ^q R _V	15161.81	Z (12)
								D \rightarrow X, ^r	continuum	
C $1\Sigma_g^+$	3p σ 157415	1653.43	Z 41.0 ₄ ^s	7.052	0.215 ^t	5.08 ^u	1.092 ₉	C \rightarrow A, R	10945.50	Z (11) (39)
B $1\pi_g$	2p π 149914	1765.76	Z 34.39 ^v	7.403 ^w	0.216 ^w	5.02 ^w	1.066 ₇	(B - A)	3501.5 ^x	
A $1\Sigma_u^+$	2s σ 146365 ^y	1861.3 ₃	Z 35.28 ^z	7.778 ₉	0.216 ₆ ^{a'}	5.44	1.0406	A \leftrightarrow X, ^{b'}	147279 ^{c'}	(8) (18) (22)
								Hopfield continuum		(38)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}_2$ (continued)										
X $1\Sigma_g^+$	0	Repulsive potential with very small well ($D_e = 0.90 \text{ meV}$).					2.97 ^d			

He₂: ^aAverage of Π^- and Δ^- as given by (39).

^bAverage of Σ^+ , Π^+ , Δ^+ as given by (39).

^cThese constants refer to Π^- and Δ^- which are less affected by ℓ -uncoupling.

^dRefers to $N=1$.

^e(50) give average effective constants for the four interacting components $J(1\Delta_u^+, 1\Pi_u^+, 1\Sigma_u^+)$ and $H 1\Sigma_u^+$.

^fSee ^mp. 295.

^gThese constants are corrected for ℓ -uncoupling effects.

^h $\gamma_e = -0.0045$.

ⁱ $D_1 = 5.26 \times 10^{-4}$, $H_0 = 2.18 \times 10^{-8}$.

^j $D_1 = 5.26 \times 10^{-4}$, $H_0 = 1.97 \times 10^{-8}$.

^k $D_1 = 5.29 \times 10^{-4}$.

^l $\omega_e y_e = -0.023$.

^mThe rotational constants refer to Π^- (36); $B(\Pi^-) - B(\Pi^+) \approx +0.044$.

ⁿ $\gamma_e = -0.00227$.

^o $\gamma_e = -0.0059$.

^p $\beta_e = +0.19 \times 10^{-4}$.

^qFranck-Condon factors (25).

^rThe weak maximum near 676 \AA in the Hopfield continuum is ascribed by (37) to the transition $D \rightarrow X$.

^s $\omega_e y_e = +0.3549$, $\omega_e z_e = -0.1315$. Calculations of (47) give a potential hump of 0.22 eV at 2.09 \AA ; see also (59)

^t $\gamma_e = -0.0111$. | and (60).

^u $\beta_e = +0.10 \times 10^{-4}$; $H_0 = 1.72 \times 10^{-8}$, ...

^v $\omega_e y_e = -0.0267$ (12).

^w B_e refers to Π^- ; $B(\Pi^-) - B(\Pi^+) = +0.019$; $\gamma_e = -0.0015$,

^xFrom (39). | $\beta_e = +0.05 \times 10^{-4}$ (12).

^yRKR potential curve (34)[see also (39)]; ab initio potential (42). The latter gives vibrational and rotational levels in good agreement with the experimental values. (8) have established, from the absorption and emission bands near 600 \AA , a potential maximum of 0.059 eV in the $A 1\Sigma_u^+$ state. Theoretical work by (15)(16)(47) gives maxima of 0.084, 0.153, 0.061 eV, respectively; see also (59)(60).

^z $\omega_e y_e = -0.136$ (36).

^a $\gamma_e = -0.00273$ (36).

^bTransitions from the low vibrational levels of $A 1\Sigma_u^+$ to $X 1\Sigma_g^+$ give rise to the Hopfield continuum; see MOLSPEC 1, 404. Transitions from the high vibrational levels as well as the continuous range of energy levels of $A 1\Sigma_u^+$ to $X 1\Sigma_g^+$ give rise to diffuse bands near 600 \AA observed in emission (18) (22) and absorption (8)(38) with quite different intensity distribution. See also (6)(37) and (31)(52)(54). Observed absorption coefficients near 600 \AA (38) agree fairly well with those predicted by (41).

^cEnergy of the $v=0, N=0$ level of $A 1\Sigma_u^+$ relative to $\text{He}(^1S) + \text{He}(^1S)$, calculated from the corresponding value for a $3\Sigma_u^+$ by (continued p. 299)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}_2^+$		$\mu = 2.0011645$	$D_0^0 = 2.365 \text{ eV}^a$						NOV 1976 A	
A $^2\Sigma_g^+$		Repulsive state arising from $\text{He}(1^1\text{S}) + \text{He}^+(1^2\text{S})$. ^b								(4)(6)(8)
X $^2\Sigma_u^+$	0	1698.5^c	35.3	7.211^c	0.224	5.1	1.080_8		(9)(10)(14)	
$^4\text{He}_2^{++}$		$\mu = 2.0010273$							NOV 1976 A	
X $^1\Sigma_g^+$		Calculations of excited states by (3)(5). (3295) ^d					$(0.704)^e$		(1)(2)(7)	

He_2^+ , He_2^{++} :

^aFrom the theoretical $D_e = 2.469 \pm 0.006 \text{ eV}$ (12). From He-He⁺ differential scattering cross sections (6) and (13) obtain $D_e = 2.34$ and 2.55 eV , respectively.

^bThe potential functions of several excited states have been calculated by (4)(11). A $^2\Sigma_g^+$, the lowest $^2\Sigma_g^+$ state, has a very small van der Waals minimum at 5.3 \AA and a hump near 0.8 \AA caused by an avoided crossing with the second lowest $^2\Sigma_g^+$ state; see (8). The states $^4\Sigma_u^+$, $^2\Sigma_g^+$, $^2\Sigma_u^+$ arising from $\text{He}(2^3\text{S}) + \text{He}^+(1^2\text{S})$ are found to have minima with $D_e \approx 1.1$, 0.57 , 0.46 eV , respectively; several other states are purely repulsive.

^cConstants obtained by extrapolation from the $n\pi\text{ Ryd-berg}$ series of He_2 ; they agree with values derived from the theoretical potential function of (4) and (8).

^dTheoretical value (2).

^eThe theoretical potential function according to (2)(7) shows a local minimum at 0.704 \AA and 69600 cm^{-1} above $\text{He}^+ + \text{He}^+$, separated from this limit by a maximum at 1.151 \AA and

82200 cm^{-1} . He_2^{++} has not yet been found mass-spectrometrically, nor has its spectrum been observed.

(1) Kolos, Roothaan, RMP 32, 219 (1960).

(2) Fraga, Ransil, JCP 37, 1112 (1962).

(3) Browne, JCP 42, 1428 (1965).

(4) Browne, JCP 45, 2707 (1966).

(5) Jennings, JCP 46, 2442 (1967).

(6) Olson, Mueller, JCP 46, 3810 (1967).

(7) Conroy, Bruner, JCP 47, 921 (1967).

(8) Gupta, Matsen, JCP 47, 4860 (1967).

(9) See ref. (23) of He_2 .

(10) See ref. (30) of He_2 .

(11) Bardsley, PR A 3, 1317 (1971).

(12) Liu, PRL 27, 1251 (1971).

(13) Weise, Mittmann, Ding, Henglein, ZN 26 a, 1122 (1971).

(14) See ref. (46) of He_2 .

He₂ (continued):

adding the energy difference $\Delta v = 2343.91 \pm 0.05 \text{ cm}^{-1}$ as determined by (62) from singlet-triplet anticrossings. Optical measurements give $\Delta v = 2344.1 \text{ cm}^{-1}$ (30). The relative position of the levels is much more accurately known than their absolute values.

^dFrom differential elastic scattering measurements (45)(66).

- (1) Dieke, ZP 57, 71 (1929).
- (2) Dieke, Imanishi, Takamine, ZP 57, 305 (1929).
- (3) Jevons, "Band Spectra of Diatomic Molecules", Physical Society, London (1932).
- (4) Dieke, Robinson, PR 80, 1 (1950).
- (5) Hepner, Herman, CR 243, 1504 (1956).
- (6) Tanaka, Jursa, LeBlanc, JOSA 48, 304 (1958).
- (7) Poshusta, Matsen, PR 132, 307 (1963).
- (8) Tanaka, Yoshino, JCP 39, 3081 (1963); 50, 3087 (1969).
- (9) Mulliken, PR A 136, 962 (1964).
- (10) Browne, PR A 138, 9 (1965).
- (11) Ginter, JCP 42, 561 (1965).
- (12) Ginter, JMS 17, 224 (1965).
- (13) Ginter, JMS 18, 321 (1965).
- (14) Gloersen, Dieke, JMS 16, 191 (1965).
- (15) Allison, Browne, Dalgarno, PPS 89, 41 (1966).
- (16) Scott, Greenawalt, Browne, Matsen, JCP 44, 2981 (1966).
- (17) Ginter, JCP 45, 248 (1966).
- (18) Mies, Smith, JCP 45, 994 (1966).
- (19) Callear, Hedges, Nature 215, 1267 (1967).
- (20) Ludlum, Larson, Caffrey, JCP 46, 127 (1967).
- (21) Klein, Greenawalt, Matsen, JCP 47, 4820 (1967).
- (22) Smith, JCP 47, 1561 (1967); 49, 4817 (1968).
- (23) Ginter, Ginter, JCP 48, 2284 (1968).
- (24) Murrell, Shaw, MP 15, 325 (1968).
- (25) Zhirnov, Shadrin, OS(Engl. Transl.) 24, 478 (1968).
- (26) Gupta, Matsen, JCP 50, 3797 (1969).
- (27) Murrell, MP 16, 601 (1969).
- (28) Alexander, JCP 52, 3354 (1970).
- (29) Bruch, McGee, JCP 52, 5884 (1970).
- (30) Ginter, Battino, JCP 52, 4469 (1970).
- (31) Michaelson, Smith, CPL 6, 1 (1970).
- (32) DONNSPEC (1970).
- (33) Schaefer, McLaughlin, Harris, Alder, PRL 25, 988 (1970).
- (34) Smith, Chow, JCP 52, 1010 (1970).
- (35) Bennewitz, Busse, Dohmann, CPL 8, 235 (1971).
- (36) Brown, Ginter, JMS 40, 302 (1971).
- (37) Chow, Smith, JCP 54, 1556 (1971).
- (38) Chow, Smith, Waggoner, JCP 55, 4208 (1971).
- (39) Ginter, in (32).
- (40) Liu, PRL 27, 1251 (1971).
- (41) Sando, Dalgarno, MP 20, 103 (1971).
- (42) Mukamel, Kaldor, MP 22, 1107 (1971).
- (43) McLaughlin, Schaefer, CPL 12, 244 (1971).
- (44) Bennewitz, Busse, Dohmann, Oates, Schrader, ZP 253, 435 (1972); PRL 29, 533 (1972).
- (45) Farrar, Lee, JCP 56, 5801 (1972).
- (46) Ginter, Brown, JCP 56, 672 (1972).
- (47) Guberman, Goddard, CPL 14, 460 (1972).
- (48) Gupta, MP 23, 75 (1972).
- (49) Sando, quoted by (46).
- (50) Brown, Ginter, JMS 46, 256 (1973).
- (51) Liu, McLean, JCP 59, 4557 (1973).

(continued p. 301)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-2}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}^40\text{Ar}$ X $1\Sigma^+$ 0		$\mu = 3.6382034_6$		$D_e^0 = 0.0024 \text{ eV}^a$ Only $v=0$ is bound; see (6)			3.51^a	Translational sp. ^b		SEP 1976 A (1)
$^4\text{He}^40\text{Ar}^+$ A $2\Sigma^+$ $X_2 (\frac{1}{2})$ 1500 $X_1 (\frac{1}{2}, \frac{3}{2})$ 0 }				$D_e(A^2\Sigma^+) = 0.19 \text{ eV}^a$ Two broad groups of bands with partially resolved rotational structure. No vibrational assignments. Arising from He + $\text{Ar}^+(^2P$ ground state splitting 1432 cm^{-1}).				$A \rightarrow X_2, ^b V$ 68630 $A \rightarrow X_1, ^b V$ 70130 ^c		SEP 1976 (2)*
$^4\text{He}^1\text{H}$ X $2\Sigma^+$		$\mu = 0.80510570$		$D_e^0 = (0.003) \text{ eV}^a$ Excited states derived from $\text{He}(1s^2) + \text{H}(2s, 2p)$ and from $\text{He}(1s2s, 1s2p) + \text{H}(1s)$ have been calculated by (1)(4) and (3), respectively. Several of these states have dissociation energies of the order of 2 eV. Calculated potential function (3); comparison with H-He scattering results (2).				Translational sp. ^b		SEP 1976 A
$^4\text{He}^1\text{H}^+$ A $1\Sigma^+$ (104707) a $3\Sigma^+$ (104273) X $1\Sigma^+$ 0				$D_0^0 = (1.8450) \text{ eV}^a$ Several other excited 1Σ states calculated by (8), lowest $1, 3\Pi$ states by (2); see also (1). [(157.5)] ^b [(297.6)] (3228.4) (157.71) ^d (34.887) ^e (2.636 ₂) ^d (1.61) (0.7743)			(2.9) (2.3 ₆) (0.7743)	(A-X) ^c (103244) (a-X) (102847)		(12) (12) (11)

HeAr: ^aFrom molecular beam scattering measurements; average of values given by (4) and (5).

^bDipole moment function from ab initio calculations (2) and from translational absorption spectra (3).

(1) Bosomworth, Gush, CJP 43, 751 (1965)

(2) Matcha, Nesbet, PR 160, 72 (1967).

(3) Bar-Ziv, Weiss, CPL 19, 148 (1973).

(4) Chen, Siska, Lee, JCP 59, 601 (1973).

(5) Smith, Rulis, Scoles, Aziz, Duquette, JCP 63, 2250 (1975).

(6) Bobetic, Barker, JCP 64, 2367 (1976).

HeAr⁺: ^aFrom He⁺-off-Ar elastic scattering data (1).

^bA → X₁ is stronger than A → X₂.

^cThe transition energy is close to the difference of He + Ar⁺ and He⁺ + Ar which is 71201 cm⁻¹. This agreement, together with the characteristic splitting of the lower states, makes the explanation by (2) of the observed bands as a charge transfer spectrum very convincing.

(1) Weise, BBPC 77, 578 (1973).

(2) Tanaka, Yoshino, Freeman, JCP 62, 4484 (1975).

He¹H: ^aTheoretical value (3); 0.0007₃ eV (5) seems less likely to be correct considering that D_e⁰(He₂) = 0.00090 eV.

^bTheoretical intensity distrib.(5); no experimental data.

(1) Michels, Harris, JCP 39, 1464 (1963).

(2) Fischer, Kemmey, JCP 53, 50 (1970).

(3) Miller, Schaefer, JCP 53, 1421 (1970).

(4) Slocomb, Miller, Schaefer, JCP 55, 926 (1971).

(5) Ulrich, Ford, Browne, JCP 57, 2906 (1972).

He¹H⁺: ^aTheoretical value (11) from the potential function of (9) (10); D_e⁰ = 2.0402 eV. Proton scattering by He gives D_e⁰ = 2.0₀ eV (4).

^bΔG(3/2) = 78.8, zero-point energy 112.1, derived by (12)

He¹H⁺ (continued):

from the potential function of (9); see also (8).

^cFranck-Condon factors for bound-continuum transitions (3).

^dω_ev_e = + 0.454, γ_e = - 0.0305. A number of quasi-bound levels (below the centrifugal barrier) have been observed (5) in the momentum distribution of protons formed in the predissociation of HeH⁺; they have been calculated by (6) (7)(10)(11).

^eu_{el} (referred to the center of mass) = 1.66 D (11).

(1) Michels, JCP 44, 3834 (1966).

(2) Hoyland, JCP 47, 49 (1967).

(3) Sizun, Durup, MP 22, 459 (1971).

(4) Weise, Mittmann, Ding, Henglein, ZN 26 a, 1122 (1971).

(5) Schopman, Fournier, Los, Physica 63, 518 (1973).

(6) Peek, Physica 64, 93 (1973).

(7) Bernstein, CPL 25, 1 (1974).

(8) Green, Michels, Browne, Madsen, JCP 61, 5186 (1974).

(9) Kolos, IJQC 10, 217 (1976).

(10) Kolos, Peek, CP 12, 381 (1976).

(11) Dabrowski, Herzberg, N.Y. Acad. Sci. (II) 38, 14 (1977).

(12) Dabrowski, Herzberg, unpublished.

He₂ (continued):

(52) Mukamel, Kaldor, MP 26, 291 (1973).

(53) Bertoncini, Wahl, PRL 25, 991 (1970); JCP 58, 1259

(54) Peatman, Wu, CP 2, 335 (1973). | (1973).

(55) Beck, Nicolaides, Musher, PR A 10, 1522 (1974).

(56) Kleinman, Wolfsberg, JCP 61, 4366 (1974).

(57) Foreman, Rol, Coffin, JCP 61, 1658 (1974).

(58) Lichten, McCusker, Vierima, JCP 61, 2200 (1974).

(59) Andresen, Kuppermann, MP 30, 997 (1975).

(60) Guberman, Goddard, PR A 12, 1203 (1975).

(61) Chapman, PR A 12, 2333 (1975).

(62) Miller, Freund, Zegarski, Jost, Lombardi, Derouard, JCP 63, 4042 (1975).

(63) Poulat, Larsen, Novaro, MP 30, 645 (1975).

(64) Snook, Spurling, JCS FT II 71, 852 (1975).

(65) Vierima, JCP 62, 2925 (1975).

(66) Burgmans, Farrar, Lee, JCP 64, 1345 (1976).

(67) Orth, Ginter, JMS 61, 282 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}^1\text{H}^{++}$		$D_e(A^2\Sigma^+) = (0.849_5) \text{ eV}^a$ Potential functions of several states calculated by (1)(2). Only $A^2\Sigma^+$ [from $\text{H}(1s) + \text{He}^{++}$] has a minimum. Satisfactory agreement with charge exchange experiments [$\text{He}^{++} + \text{H} \rightarrow \text{He}^+ + \text{H}^+$; (2)].								SEP 1976 A
A $^2\Sigma^+$	(322378) ^a	(950) ^a	(39) ^a				(2.05 ₉) ^a			
X $^2\Sigma^+$		Repulsive state (corresponding to $\text{He}^+ + \text{H}^+$).								
$^4\text{He}^{(84)}\text{Kr}$		$(\mu = 3.8203705) \quad D_e^0 = 0.0021_3 \text{ eV}^a$ Doubtful whether any level other than $v=0$ is bound (2).						3.75 ^a		SEP 1976 A
X $^1\Sigma^+$										
$^4\text{He}^{(84)}\text{Kr}^+$		$D_e(A^2\Sigma^+) = 0.22 \text{ eV}^a$ Two broad groups of partially resolved bands, no vibr. assignments. Arising from $\text{He} + \text{Kr}^+ (^2P \text{ ground state splitting } 5371 \text{ cm}^{-1})$.						$A \rightarrow X_2, \quad V_R \quad 78370_b$ $A \rightarrow X_1, \quad 83820_b$		SEP 1976 (2)*
A $^2\Sigma^+$										
$X_2 (\frac{1}{2})$	5450									
$X_1 (\frac{1}{2}, \frac{3}{2})$	0									
$^4\text{He}^{(20)}\text{Ne}$		$(\mu = 3.3349306_8) \quad D_e^0 = 0.0012_3 \text{ eV}^a; D_0^0 = (0.0002_3) \text{ eV, see (4).}$ Similar but unclassified bands near other strong Ne lines.								SEP 1976 A
F		[120] ^b	Progression of five bands converging to $3d'[\frac{3}{2}]1_u$ of Ne.					$F \leftarrow X,^c$	162050	(2)
E		[40] ^b	Progression of six bands converging to $3d[\frac{1}{2}]1_u$ of Ne.					$E \leftarrow X,^c$	161340	(2)
D		[30] ^b	Progression of four bands converging over a maximum to $4s'[\frac{1}{2}]1_u$ of Ne.					$D \leftarrow X,^c$	159590	(2)
C		[100] ^b	Progression of six bands converging to $4s'[\frac{1}{2}]1_u$ of Ne.					$C \leftarrow X,^d$	V 159050	H (2)
B		[40] ^b	Progression of four bands converging over a maximum to $4s[\frac{3}{2}]1_u$ of Ne.					$B \leftarrow X,^c$	158860	(2)
A		[150] ^b	Progression of three bands converging to $4s[\frac{3}{2}]1_u$ of Ne.					$A \leftarrow X,^d$	V 158440	H (2)
X $^1\Sigma^+$	0	Only $v=0$ is bound; see (4).					3.21 ^a	e		

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^4\text{He}^{20}\text{Ne}^+$		$D_0^0 = 0.69_2 \text{ eV}^a$ RKR potential curves (7), theoretical potential functions (4).								APR 1978
B $^2\Sigma^+$	(30233)	152.649 Z	21.718 ^b	0.72116 ^c	0.08978 ^d	[0.855] ^e	2.6475 ₂	B \rightarrow X, R	$v(0-6) = 24970.73^f$ Z	} (1)* (2) (6)* (7)*
A ₂ $^2\Pi_{1/2}$	(6649)	[129.69] Z		[0.86571] ^g	h	[1.592] ^e	2.3186	B \rightarrow A ₂ , R	23590.23 Z	
A ₁ $^2\Pi_{3/2}$		Not yet observed.								
X $^2\Sigma^+$	0	(1308.3) ^f	(84.8) ⁱ	(2.991) ^j	(0.191) ^k	$D_6 = 2.098^e$	(1.300)			

He¹H⁺⁺: ^aTheoretical values (1); T_e is relative to He⁺ + H⁺.

- (1) Bates, Carson, PRS A 234, 207 (1956).
(2) Piacentini, Salin, JP B 7, 1666 (1974).

HeKr: ^aFrom molecular beam scattering measurements (1).

- (1) See ref. (4) of HeAr.
(2) See ref. (6) of HeAr.

HeKr⁺: ^aFrom He⁺-off-Kr elastic scattering data (1).

- ^bThe transition energy is close to the difference of He⁺ + Kr and He + Kr⁺ which is 85396. See ^c of HeAr⁺.
(1) See ref. (1) of HeAr⁺.
(2) See ref. (2) of HeAr⁺.

HeNe: ^aFrom molecular beam scattering measurements (3).

- ^bFirst observed ΔG , not necessarily $\Delta G(\frac{1}{2})$.
^cVery diffuse features.
^dDiffuse band heads.
^eTheoretical dipole moment function (1).

- (1)(3)(4) See ref. (2)(4)(6), resp., of HeAr.
(2) Tanaka, Yoshino, JCP 57, 2964 (1972).

HeNe⁺: ^aExtrapol. to $v=0$ from the lowest observed ground state level ($v=6$). The more accurately known $D_6^0 = 882.5 \text{ cm}^{-1}$ is based on a short extrapolation of the vibrational levels in B $^2\Sigma^+$.

HeNe⁺ (continued):

^b $w_e y_e = +1.005$. $D_0 = 292.8$, $D_e = 364.0 \text{ cm}^{-1}$ (?) confirming the less precise value from elastic scattering data [He⁺ + Ne,

^cNo spin doubling observed. A hfs splitting | see (5)].
of $\sim 0.30 \text{ cm}^{-1}$ occurs in the spectrum of $^3\text{HeNe}^+$ (7).

^d $y_e = -0.00348$.

^eFor other D_v and higher order constants see (7).

^fOnly $v''=6\dots 9$ observed because of Franck-Condon factors;
 $\Delta G''(6\frac{1}{2}, \dots) = 341.59, 233.42, 146.27$. Vibrational numbering established by the study of the spectrum of $^3\text{HeNe}^+$ (7); see

^gVery large Ω -type doubling. Rotational struc- | also (3).
ture similar to that of a $^2\Sigma^-$ state with $y_0 = +0.3047_0$.

^h $B_1 = 0.71658$.

ⁱ $w_e y_e = +(1.5)$.

^jSee ^f; $B_6\dots B_9 = 1.58983, 1.35755, 1.09037, 0.8431$. Large spin splitting, $y_6 = +0.82985$. For other y_v and higher order
^k $y_e = -(0.0038)$. | const. see (7).

(1) Oskam, Jongerius, Physica 24, 1092 (1958).

(2) Fache, CR 256, 2145 (1963).

(3) Henderson, Matsen, Robertson, JCP 43, 1290 (1965).

(4) Sidis, Lefebvre-Brion, JP B 4, 1040 (1971).

(5)(6) See ref. (1)(2), resp., of HeAr⁺.

(7) Dabrowski, Herzberg, to be published.

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻⁴ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	v ₀₀	
⁴ He(¹³²)Xe X 1Σ ⁺		(μ = 3.8847222)		D _e ⁰ = 0.0021 ₇ eV ^a D ₀ ⁰ = (0.0010 ₃) eV ^b			4.15 ^a	Translational sp.	SEP 1976 A (1)	
⁴ He(¹³²)Xe ⁺ A 2Σ ⁺ X ₂ (½) 10720 X ₁ (½, ¾) 0				D _e (A ² Σ ⁺) = 0.28 eV ^a Two broad and only partially resolved groups of indistinct band heads; no vibrational assignments. Arising from He + Xe ⁺ (² P ground state splitting 10537 cm ⁻¹).				A→X ₂ , 87800 ^b A→X ₁ , 98520 ^b	SEP 1976 (2)	
¹ H ¹ F D 1Σ ⁺ C 1Π (105820) b 3Π B 1Σ ⁺ 84776.65 A X 1Σ ⁺ 0		μ = 0.95705545		D ₀ ⁰ = 5.869 eV ^a I.P. = 16.039 eV ^b Rydberg levels converging to the ground state of HF ⁺ have been observed in the electron energy loss spectrum. Two strong bands between 104000 and 116000 cm ⁻¹ , not yet analysed. Absorption bands above 100000 cm ⁻¹ , not yet analysed. 1159.18 Z 18.005 ^c 4.0291 ^d 0.0177 ^e 1.932 ^f 2.0908 ₆ Continuous absorption starting at 60600 cm ⁻¹ . ^h 4138.32 ⁱ Z 89.88 ^j 20.9557 ^{ikl} 0.798 ^m 21.51 ⁿ 0.91680 ₈				D←X, C←X, R 105090.8 b←X, B↔X, ^g R 83304.96 Z Rot.-vibr. sp. ^{opq} Rotation sp. ^{rq} Mol. beam el. reson. ^s Mol. beam magn. reson. ^t	JAN 1977 A (44) (30) (25)(30) (25) (3)(30)* (2) (6)(7)(10)(19) (9)(11)(16) (8)(20)(26)(31) (5)	

HeXe: ^aFrom molecular beam scattering measurements (2).

^bTheoretical values from (3).

(1) Marteau, Vu, Vodar, CR B 266, 1068 (1968).

(2) See ref. (4) of HeAr.

(3) See ref. (6) of HeAr.

HeXe⁺: ^aFrom He⁺-off-Xe scattering data (1).

^bThe transition energy is close to the difference of He + Xe⁺ and He⁺ + Xe which is 100477 cm⁻¹. See ^c of HeAr⁺.

(1) See ref. (1) of HeAr⁺.

(2) See ref. (2) of HeAr⁺.

¹_{HF}: ^aFrom the limiting curve of dissociation for the ground state (30); see ^k.

^bFrom photoelectron spectra (32)(41). Earlier photoionization studies yielded 16.00₇ eV (23), a value strongly affected by the presence of autoionizing Rydberg levels in the threshold region (41). The second ionization potential (removal of a 36 electron) from the photoelectron spectrum (21)(41) is 19.118 eV in agreement with the value derived from the spectrum of HF⁺. The third and fourth ionization potentials (removal of a 26 and 16 electron, respectively) are 39.61 (38)(39) and 694.25 eV (39); these are vertical potentials from X-ray photoelectron spectra.

^c $\omega_e y_e = +0.184$; the vibrational and rotational constants were obtained from a fit to the seven lowest vibrational levels (30). See ^g.

^dRKR potential curves (4)(30).

^e $-0.000950(v+\frac{1}{2})^2 + 0.000601(v+\frac{1}{2})^3$; see ^c.

^f $+0.182 \times 10^{-4}(v+\frac{1}{2}) + 0.00551 \times 10^{-4}(v+\frac{1}{2})^2$; see ^c.

^gVery extensive band system (also called V-X) extending in absorption from 96000 to 117000, in emission from

¹_{HF} (continued);

36000 to 70000 cm⁻¹. Strong perturbations above v'=27, but bands have been identified to v'=73. The B (or V) state was also observed in the electron energy loss spectrum (44).

^h_{HF} is quite transparent to 1650 Å (2). Theoretical potential curves for three repulsive states (³ Π , ¹ Π , ³ Σ^+) arising from ground state atomic products were given by (42).

ⁱIntroduction of the Dunham correction (19) gives $\omega_e = 4138.767$ and $B_e = 20.9561$.

^j $+0.90(v+\frac{1}{2})^3 - 0.0110(v+\frac{1}{2})^4 - 0.00067(v+\frac{1}{2})^5$, $v \leq 9$ (19). A different formula for higher vibrational levels ($v \leq 19$) was derived by (3). All levels up to the last ($v=19$) are tabulated in (30).

^kFor $v=14...19$ the rotational levels break off at decreasing J on account of predissociation by rotation. A few broadened lines near these limits have been observed (30). From the limiting curve the dissociation energy 47333 ± 60 cm⁻¹ has been determined (30).

^lRKR potential curves (4)(30), Dunham potential coefficients (19)(43). Ab initio calculations of molecular constants (27)(34)(37)(42).

^m $+0.0127(v+\frac{1}{2})^2 - 0.00044(v+\frac{1}{2})^3$, from (19).

ⁿ $-0.68 \times 10^{-4}(v+\frac{1}{2}) + 0.029 \times 10^{-4}(v+\frac{1}{2})^2$, $H_e = 1.59 \times 10^{-7}$; from (19), see also (6).

^o1-0, 2-0 bands studied in absorption under high resolution by (7)(19), 3-0, 4-0, 5-0 in the photographic infrared by (1)(10). In emission, rotation-vibration bands have been studied by (6) and (40), the latter extending the chemical laser emission, first observed in the 2-1 band by (15), to $v=9$ and $\Delta v=6$. Electric discharge induced laser emission in the 3-2, 2-1, 1-0 bands, see (12)(24).

(continued on p. 307)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^2\text{H}^1\text{F}$		$\mu = 1.82104540$		$D_0^0 = 5.938 \text{ eV}^a$		$\text{I.P.} = 16.058 \text{ eV}^b$				JAN 1977
B $^1\Sigma^+$	84824.0 ^c	839.4	Z 8.90	2.1210	0.0071 ₂	0.5543 ^d	2.0891	B \rightarrow X, R 83753.8	Z	(2)
X $^1\Sigma^+$	0	2998.19 ₂ ^e	Z 45.76 ₁ ^e	11.0102 ^e	0.3017 ^e	5.94 ^e	0.91694	Rot.-vibr. sp. ^{fgh}		(1)(4)
								Rotation sp. ^h		(5)(7)(11)
								Mol. beam el. reson. ⁱ		(9)
								Mol. beam magn. reson.		(3)

²HF: ^aFrom $D_0^0(^1\text{HF})$.

^bFrom photoelectron spectra (6)(8)(14). Photoionization studies yield 16.03 eV (10).

^cLarge electronic isotope shift.

^d $\beta_e = +0.0464 \times 10^{-4}$.

^eBased on the 1-0 and 2-0 rotation-vibration bands (4);

$\gamma_e = +0.00275$, $\beta_e = -0.12 \times 10^{-4}$. Using the older measurements of (1) for $v=0,1,2$ and their own measurements of the B-X system at high v (2) obtain:

$$G(v) = 3001.008(v+\frac{1}{2}) - 47.969(v+\frac{1}{2})^2 + 0.58504(v+\frac{1}{2})^3 \\ - 0.028102(v+\frac{1}{2})^4 + 9.9959 \times 10^{-4}(v+\frac{1}{2})^5 \\ - 2.0290 \times 10^{-5}(v+\frac{1}{2})^6 \quad (v \leq 24);$$

$$B_v = 11.00375 - 0.30362(v+\frac{1}{2}) + 0.0038495(v+\frac{1}{2})^2 - 1.7593 \times 10^{-4}(v+\frac{1}{2})^3 + 9.1687 \times 10^{-6}(v+\frac{1}{2})^4 - 3.1044 \times 10^{-7}(v+\frac{1}{2})^5;$$

also higher terms in the expression for D_v . (11) obtain from the submillimeter microwave spectrum $B_0 = 10.860346$.

^fLaser emission in the 4-3, 3-2, 2-1, 1-0 bands in transverse discharges through $D_2 + \text{SF}_6$ (12); in a chemical laser source the emission extends to $v=12$ and $\Delta v=6$ (17).

^gThe radiative lifetime of $v=1$ is 0.032 s; see (15)(16).

^hMid- and far-infrared spectra in rare-gas matrices (13).

ⁱ $\mu_{el}(v=0, J=1) = 1.81881 \text{ D}$; also nuclear quadrupole and other hyperfine coupling constants.

(1) Talley, Kaylor, Nielsen, PR 77, 529 (1950).

(2) See ref. (3) of ^1HF .

(3) Nelson, Leavitt, Baker, Ramsey, PR 122, 856 (1961).

(4) Spanbauer, Rao, Jones, JMS 16, 100 (1965).

(5) See ref. (11) of ^1HF .

(6) See ref. (18) of ^1HF .

(7) Perkins, SA A 24, 285 (1968).

(8) Brundle, CPL 7, 317 (1970).

(9) See ref. (20) of ^1HF .

(10) See ref. (23) of ^1HF .

(11) De Lucia, Helminger, Gordy, PR A 3, 1849 (1971).

(12) See ref. (24) of ^1HF .

(13) See ref. (22) of ^1HF .

(14) See ref. (32) of ^1HF .

(15) See ref. (33) of ^1HF .

(16) Bonczyk, PR A 11, 1522 (1975).

(17) See ref. (40) of ^1HF .

¹HF (continued):

^PLine strengths, collision-broadened widths, dipole moment function (28)(29)(35)(36)(40)(45). The radiative lifetime of $v=1$ [P(4) line] is 6.16 ms (33). (40) give a vibrational dipole moment matrix for $v \leq 9$ based on intensity measurements in chemical laser emission.

^QRotation and rotation-vibration spectra in rare-gas matrices (22).

^RLaser emission in the pure rotation spectrum (13).

^S $\mu_{el}(v=0, J=1) = 1.82618 \text{ D}$ (20)(26); $g_J = 0.7410$, quadrupole moment $\theta = 2.36 \times 10^{-26} \text{ esu cm}^2$ (31); also nuclear spin - rotation and other hyperfine structure constants.

^TNuclear reorientation spectrum.

- (1) Naudé, Verleger, PFS A 63, 470 (1950).
- (2) Safary, AP(Paris) 2, 203 (1954).
- (3) Johns, Barrow, PRS A 251, 504 (1959).
- (4) Fallon, Vanderslice, Mason, JCP 32, 698; 33, 944 (1960).
- (5) Baker, Nelson, Leavitt, Ramsey, PR 121, 807 (1961).
- (6) Mann, Thrush, Lide, Ball, Acquista, JCP 34, 420 (1961).
- (7) Herget, Deeds, Gailar, Lovell, Nielsen, JOSA 52, 1113 (1962).
- (8) Weiss, PR 131, 659 (1963).
- (9) Rothschild, JOSA 54, 20 (1964).
- (10) Fishburne, Rao, JMS 19, 290 (1966).
- (11) Revich, Stankevich, DANS 170, 1376 (1966); engl. transl. DPC 170, 699 (1966).
- (12) Deutsch, APL 10, 234 (1967).
- (13) Deutsch, APL 11, 18 (1967).
- (14) Frost, McDowell, Vroom, JCP 46, 4255 (1967).
- (15) Kompa, Pimentel, JCP 47, 857 (1967).
- (16) Mason, Nielsen, JOSA 57, 1464 (1967).

- (17) Lempka, Passmore, Price, PRS A 304, 53 (1968).
- (18) Lempka, Price, JCP 48, 1875 (1968).
- (19) Webb, Rao, JMS 28, 121 (1968).
- (20) Muentert, Klemperer, JCP 52, 6033 (1970).
- (21) Berkowitz, CPL 11, 21 (1971).
- (22) Mason, Von Holle, Robinson, JCP 54, 3491 (1971).
- (23) Berkowitz, Chupka, Guyon, Holloway, Spohr, JCP 54, 5165 (1971).
- (24) Goldhar, Osgood, Javan, APL 18, 167 (1971).
- (25) Di Lonardo, Douglas, JCP 56, 5185 (1972).
- (26) Muentert, JCP 56, 5409 (1972).
- (27) Bondybey, Pearson, Schaefer, JCP 57, 1123 (1972).
- (28) Meredith, JQSRT 12, 485 (1972); Meredith, Smith, JQSRT 13, 89 (1973).
- (29) Spellicy, Meredith, Smith, JCP 57, 5119 (1972).
- (30) Di Lonardo, Douglas, CJP 51, 434 (1973).
- (31) de Leeuw, Dymanus, JMS 48, 427 (1973).
- (32) Walker, Dehmer, Berkowitz, JCP 59, 4292 (1973).
- (33) Hinchey, JOSA 64, 1162 (1974).
- (34) Krauss, Neumann, MP 27, 917 (1974).
- (35) Lie, JCP 60, 2991 (1974).
- (36) Rimpel, ZN 29 a, 588 (1974).
- (37) Meyer, Rosmus, JCP 63, 2356 (1975).
- (38) Banna, Shirley, JCP 63, 4759 (1975).
- (39) Shaw, Thomas, PR A 11, 1491 (1975).
- (40) Sileo, Cool, JCP 65, 117 (1976).
- (41) Guyon, Spohr, Chupka, Berkowitz, JCP 65, 1650 (1976).
- (42) Dunning, JCP 65, 3854 (1976).
- (43) Ogilvie, Koo, JMS 61, 332 (1976).
- (44) Salama, Hasted, JP B 2, L333 (1976).
- (45) Yardley, Balint-Kurti, MP 31, 921 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^3\text{H}^9\text{F}$ X $1\Sigma^+$	0	$\mu = 2.6028413_9$ 2508.5_4^b	$D_0^0 = 5.968 \text{ eV}^a$ Z 32.5_4^b	7.692	0.176^c	[2.6]	0.9176	Rotation-vibration b.	JAN 1977 (1)	
$^1\text{H}^9\text{F}^+$ A $2\Sigma^+$ X $2\Pi_1$	25449.82^d 0^k	1496.07 3090.48	Z 88.42_3^e Z 88.99_6^e	11.753_6^{fg} 17.577_1^{mn}	1.0261^h 0.8863^o	$[28.8_9]^i$ $[22.0_5]^p$	1.2242 1.0011	c 678.2 eV c 23.6 eV A \rightarrow X, R 24648.91^j	JAN 1977 (5) (5) (4)	
$^2\text{H}^9\text{F}^+$ A $2\Sigma^+$ X $2\Pi_1$	25490 0^c	1080^b 2250^b	55 45.8				(A-X)	24900^b	JAN 1977	
$^1\text{H}^9\text{F}^-$ A 2Π X $2\Sigma^+$		[2860] Progression of four resonances (due to inverse preionization) in the electron transmission current. The 2Π state is derived from its "grandparent" X $2\Pi_1$ of HF^+ by the addition of a pair of $3s\sigma$ Rydberg electrons. <u>Ab initio</u> calculations (1) predict this state to be entirely repulsive.						103440^a	JAN 1977 (2)	

 ^3HF ; a From $D_0^0(^1\text{HF})$. b From the 1-0 and 2-0 rotation-vibration bands using calculated values of $w_e y_e$ and $w_e z_e$ (1). $^c y_e = +0.001_9$.(1) Jones, Goldblatt, JMS 1, 43 (1957).

$^1\text{HF}^+$: ^aAverage of two values, 27650 and 27562 cm^{-1} , the former from $D_0^0(\text{HF}) + \text{I.P.}(\text{H}) - \text{I.P.}(\text{HF})$, the latter from the predissociation in $\text{A } ^2\Sigma^+$ (see ^g).
^bSeveral excited states of HF^{++} were observed in the Auger electron spectrum of HF (5). Tentatively, the $\dots 6^2\pi^2 \text{ } ^1\Delta$ and $^1\Sigma$ states may be identified at 33.9 and 35.9 eV above $X \text{ } ^2\Pi_{3/2}(v=0)$ of HF^+ ; the $^3\Sigma$ state remains undetected.
^cFrom X-ray photoelectron spectra; satellite ("shake-up") peaks corresponding to 25-35 eV higher excitation energies than the main 16 peak were observed by (7) and attributed to simultaneous removal of a F 1s electron and excitation of a 3s or 1 π electron into a higher orbital.
^dIncludes the Y_{00} corrections in the upper and lower states; $Y_{00}'' - Y_{00}' = 2.93 \text{ cm}^{-1}$.
^e $y_e = -7.328$.
^fSpin splitting constants $\gamma(v=0\dots 3) = 0.533_9, 0.540_0, 0.566_5, 0.644$.
^gBreaking off of rotational levels at $N=3$ for $v=3$ and $N=10$ for $v=2$ because of predissociation by rotation. The predissociation limit is $27966 \pm 50 \text{ cm}^{-1}$ above $J=\frac{3}{2}, v=0$ of $^2\Pi_{3/2}$ and corresponds to dissociation into $\text{H}^+ + \text{F}(^2\Pi_{1/2})$; see, however, the discussion in (4).
^h $y_e = -0.0933$; from $v=0,1,2$ only. $B_3 = 6.741$.
ⁱ $D_1 = 31.65 \times 10^{-4}$, $D_2 = 39.3 \times 10^{-4}$;
 $H_0 = -3.2 \times 10^{-7}$, $H_1 = -11.3 \times 10^{-7}$, $H_2 = -34 \times 10^{-7}$.
^jRefers to the zero-point of the Hill-Van Vleck formula in the lower state.
^k $A(v) = -292.85 + 0.58(v+\frac{1}{2})$; see ^l.

$^1\text{HF}^+$ (continued):

^lOnly $v=0,1,2$ have been observed with high accuracy in the optical spectrum, $v=3\dots 11$ in the photoelectron sp.(6).
^mFor Λ -type doubling constants ($p \approx 0.60$) see (4).
ⁿAb initio calculations (1)(2)(3) give molecular constants in agreement with the experimental results quoted here.
^o $y_e = +0.0142$; see ^l.
 $P_{D_1} = 21.41 \times 10^{-4}$, $D_2 = 21.24 \times 10^{-4}$.
(1) Julienne, Krauss, Wahl, CPL 11, 16 (1971).
(2) See ref. (27) of ¹ HF .
(3) Raftery, Richards, JP B 5, 425 (1972).
(4) Gewurtz, Lew, Flainek, CJP 53, 1097 (1975).
(5) See ref. (39) of ¹ HF .
(6) See ref. (41) of ¹ HF .
(7) Martin, Mills, Shirley, JCP 64, 3690 (1976).

$^2\text{HF}^+$: ^aFrom $D_0^0(\text{DF}) + \text{I.P.}(\text{D}) - \text{I.P.}(\text{DF})$; from $D_0^0(\text{HF}^+)$ one obtains 3.473 eV.

^bFrom the photoelectron spectrum of DF (1)(2)(3). The optical spectrum of DF^+ has not yet been analysed.

^c $A = -266 \text{ cm}^{-1}$, from incompletely resolved photoelectron peaks (3).

(1) See ref. (21) of ¹ HF .
(2) See ref. (32) of ¹ HF .
(3) See ref. (41) of ¹ HF .

$^1\text{HF}^-$: ^aEnergy relative to HF, $X \text{ } ^1\Sigma^+(v=0)$.

(1) See ref. (27) of ¹ HF .
(2) Spence, Noguchi, JCP 63, 505 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (Å)	Observed Transitions		References	
								Design.	ν_{00}		
$(^{180})\text{Hf}(^{79})\text{Br}$		$(\mu = 54.859052_6)$ Three sequences of R shaded bands in emission at 15860, 16110 (0-0), and (16345) cm^{-1} .							JAN 1975 (1)		
$(^{180})\text{Hf}(^{127})\text{I}$		$(\mu = 74.420556)$ Complex groups of emission bands in the regions 19700 - 20300 and 20450 - 20750 cm^{-1} . Long 0-0 sequence of R shaded bands in emission.						R 14559.7 H	JAN 1975 (1) (2)		
$^{180}\text{Hf}(^{160})$		$\mu = 14.6892328_7$ $D_0^0 = 8.19 \text{ eV}^a$ I.P. = 7.5_5 eV^b							JAN 1975 A		
J						$[0.3719]^{cd}$		$[1.756_7]$	$J \rightarrow x_3,^c \text{ R } 22655.82 \text{ Z}$	(1)* (3)(6)	
H						$[0.3699]^{cd}$		$[1.761_4]$	$H \rightarrow x_2,^c \text{ R } 21239.87 \text{ Z}$	(1)* (6)	
C	$x_1 + 19719.3$	852.5	H^Q	4.1		$[0.3696]^c$	$[3.0]$	$[1.762_1]$	$C \rightarrow x_1,^c \text{ R } 19682.94 \text{ Z}$	(1)* (6)	
x_3		$(945)^e$		(5)		$[0.3788]^c$	$[2.6]$	$[1.740_6]$			
x_2						$[0.3781]^c$	$[2.6]$	$[1.742_2]$			
x_1	x_1	925.0	H^Q	3.5		$[0.3776]^c$	$[2.8]$	$[1.743_3]$			
G	$1\Sigma(+)$	30090.0	$[852.29]$	Z	(3.7_1)	0.370106	0.002071	$[2.764]^f$	1.76090_4	$G \leftrightarrow X,^g \text{ R } 30032.71 \text{ Z}$	(1)* (3)(6)
F	$1\Sigma(+)$	27413.59	849.40	Z	3.67	0.36563	0.00188	2.702^h	1.7716_5	$F \leftrightarrow X,^g \text{ R } 27351.14 \text{ Z}$	(1)* (3)(6)*
E	1Π	25230.94	866.93	Z^i	3.68	0.36928^j ℓ	0.00198	2.69	1.7636	$E \leftrightarrow X,^g \text{ R } 25177.25^i \text{ Z}$	(1)* (3)(6) (7)
D	1Π	23554.41	872.60	Z^i	3.31	0.36912^k ℓ	0.00182	2.624^m	1.7642	$D \leftrightarrow X,^g \text{ R } 23503.65^i \text{ Z}$	(1)* (3)(6)* (7)
B	$1\Pi^o$	17562.22	907.01	Z^i	3.38	0.36837^j	0.001800	2.631^n			
						0.378060^k	0.001852	2.63			
						0.377537^j	0.001848	2.618^p	1.7429	$B \leftrightarrow X,^g \text{ R } 17528.65^i \text{ Z}$	(1)* (3)(4) (6)(7)
A	$1\Sigma(+)^o$	16616.92	914.24	Z	3.38	0.377985	0.001827	2.587^q	1.74245_4	$A \leftrightarrow X,^g \text{ R } 16586.96 \text{ Z}$	(1)* (3)(6) (7)
X	$1\Sigma(+)$	0	974.09	Z	3.228	0.386537	0.001724	2.438^r	1.72307_1	s	

HfBr: (1) Savithry, Rao, Rao, Physica 62, 400 (1973).

HfI: (1) Savithry, Rao, Rao, CS 40, 516 (1971).
(2) Savithry, Rao, Rao, CS 42, 533 (1973).

HfO: ^aThermochemical value (mass-spectrom.)(9). See also (2).

^bElectron impact appearance potential (8).

^cP, Q, and R branches. No Λ -type doubling observed.

The three systems are probably subsystems of a triplet - triplet transition, possibly $^3\phi - ^3\Delta$ [see (5)].

^d $v=0$ perturbed by state of smaller B value.

^eFrom the fluorescence spectrum of HfO in a Ne matrix (3).

^f $D_1 = 3.73 \times 10^{-7}$, perturbed.

^gAbsorption spectra of HfO in solid inert gas matrices; see (3).

^h $A_e = + 0.023 \times 10^{-7}$.

ⁱThese band origins do not conform to the usual convention adopted in these tables. Subtract B_v in order to obtain zero lines.

^jf levels.

^ke levels.

^lPerturbations between D and E.

^m $A_e = + 0.032 \times 10^{-7}$.

ⁿ $A_e = + 0.019 \times 10^{-7}$.

^oPossibly $^3\Pi_0$ and $^3\Pi_1$; see (5).

^p $A_e = + 0.009 \times 10^{-7}$.

^q $A_e = + 0.016 \times 10^{-7}$.

^r $A_e = + 0.006 \times 10^{-7}$.

^sIR spectrum of HfO trapped in Ne matrix (3).

HfO (continued):

(1) Gatterer, Junkes, Salpeter, Rosen, METOX.

(2) Panish, Reif, JCP 38, 253 (1963).

(3) Weltner, McLeod, JPC 62, 3488 (1965).

(4) Edvinsson, Naturw. 53, 177 (1966).

(5) Edvinsson, Dissertation (Stockholm, 1971). USIP Report 71-09.

(6) Edvinsson, Nylén, PS 3, 261 (1971).

(7) Wentink, Spindler, JQSRT 12, 1569 (1972).

(8) Rauh, Ackermann, JCP 60, 1396 (1974).

(9) Ackermann, Rauh, JCP 60, 2266 (1974).

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻⁸ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	v ₀₀	
(200,202) Hg ₂		(μ = 100.482247)	0.06 ₅ < D ₀ ⁰ < 0.09 ₁ eV ^a	9.39 < I.P. < 9.61 eV ^b						JAN 1975 A
		Numerous bands and continua in absorption and emission from 19000 to 71000 cm ⁻¹ . Literature before 1938 reviewed in (6); details concerning the 2540 Å (39353 cm ⁻¹) band in (7). ^c - See also HgO.								(6)
		Large number of additional emission features reported by (8) whose tentative vibrational assignments in the regions 21000 - 22800 and 18800 - 20100 cm ⁻¹ suggest ω _e ' = 122, ω _e 'x _e ' = 0.6; ω _e " = 145, ω _e "x _e " = 0.5, and ω _e ' = 121, ω _e " = 141, ω _e "x _e " = 0.5,						22152 19615		(8) (8) (2)(3)(4) (10)
X 1Σ _g ⁺	0	(36)					(3.3)			
(200,202) Hg ₂ ⁺ ?			0.91 < D ₀ ⁰ < 1.11 eV ^a							JAN 1975
		Group of bands near 40300 cm ⁻¹ .								(1)(2)
(202) Hg ⁴⁰ Ar		(μ = 33.3614163)								JAN 1975 A
		Molecular features associated with the Hg resonance line at 2537 Å (39412 cm ⁻¹), observed in emission and absorption by (1)(2)(3)(4)(10). See also the discussions by (7)(8)(9). Calculated constants for the ground state in (5)(6)(7).								
202 Hg ⁴⁰ Ar ⁺			D ₀ ⁰ = (0.20) eV							JAN 1975
A (J _a = 5/2) _{1/2}	35444.5 ^a	104.5	H	1.5	0.05789 ^b	0.00076	6.95 ^c	2.954 ₄	A → X, R _v 35447.2	H (1)* (2)(3)
X 2Σ ⁺	0	99.0	H	1.5	[0.06142]		[9.7 ₈]	[2.868 ₃]		
(202) Hg ⁸¹ Br		(μ = 57.771192)	D ₀ ⁰ = 0.71 eV							JAN 1975 A
E (40720)	(166)	(1.1)							E → X, ^a (40710)	(7)
D (2Π _{3/2})	38574.4	228.5 ^b	H	0.950					D ↔ X, v 38595.5	H (1)(5)*(13)*

Hg₂: ^aThermochemical value (1)(2)(4), disregarding corrections for rotation suggested by (9) which in our view do not apply.

^bFrom (5).

^cFor radiative lifetimes of the upper states of the 3350 Å (29840 cm⁻¹) and 4850 Å (20610 cm⁻¹) emissions see (11)(12)(13).

- (1) Koernicke, ZP 33, 219 (1925).
- (2) Kuhn, Freudenberg, ZP 76, 38 (1932).
- (3) Ekstein, Magat, CR 199, 264 (1934).
- (4) Kuhn, PRS A 158, 230 (1937).
- (5) Arnot, M'Ewen, PRS A 165, 133 (1938).
- (6) Finkelburg, "Kontinuierliche Spektren", Springer (Berlin, 1938).
- (7) Mrozowski, PR 76, 1714 (1949).
- (8) Takeyama, JSHU A 15, 235 (1952).
- (9) Winans, Heitz, ZP 133, 291 (1952); 135, 406 (1953).
- (10) Epstein, Powers, JPC 57, 336 (1953).
- (11) Ladd, Freeman, McEwan, Claridge, Phillips, JCS FT II 69, 849 (1973).
- (12) Phaneuf, Skonieczny, Krause, PR A 8, 2980 (1973).
- (13) Skonieczny, Krause, PR A 9, 1612 (1974).

Hg₂⁺: ^aFrom (I.P.)_{Hg} and (I.P. - D₀⁰)_{Hg₂} [see ref. (5) of Hg₂].

- (1) Winans, PR 42, 800 (1932).
- (2) See ref. (7) of Hg₂.

- HgAr: (1) Oldenberg, ZP 47, 184 (1928); 55, 1 (1929).
(2) Kuhn, Oldenberg, PR 41, 72 (1932).
(3) Kuhn, PRS A 158, 212 (1937).
(4) Preston, PR 51, 298 (1937).
(5) Heller, JCP 9, 154 (1941).
(6) Legowski, BAPS(MAP) 6, 127 (1958).
(7) Michels, De Kluiver, Ten Seldam, Physica 25, 1321 (1959).
(8) Fiutak, Frackowiak, BAPS(MAP) 11, 175 (1963).
(9) Behmenburg, ZN 27 a, 31 (1972).
(10) Kielkopf, Miller, JCP 61, 3304 (1974).

HgAr⁺: ^aThe observed isotope shifts closely parallel those of the corresponding transition in Hg⁺, i.e. 5d⁹6s² 2D_{5/2} → 5d¹⁰6s 2S_{1/2}.

^bLarge Ω-type doubling, Δv_{fe} = +p_v(J+½) - ... where p_v = +5.30 B_v. Theory (3) predicts p ≈ +6B.

^cβ_e = +0.23 × 10⁻⁸.

- (1) Santaram, Winans, CJP 44, 1517 (1966).
- (2) Bridge, CC (1970), p. 358; JMS 42, 370 (1972).
- (3) Hougen, JMS 42, 381 (1972).

HgBr: ^aHeadless diffuse bands.

^bConstants for ²⁰²Hg⁸¹Br.

(continued p. 315)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(202) Hg ⁸¹ Br (continued)										
C (² Π _{1/2})	34722.0	278.6 ^c	H 1.82					C ↔ X, V	34767.5 ^c H	(1)(2)(6)(8) (12)*(13)*
B ² Σ ⁺	23485.0	135.075	H 0.275					B → X, R	23459.5 H	(3)(9)(11)*
X ² Σ ⁺	0	186.47	H 0.9665 ^d							(11)
(202) Hg ³⁵ Cl										
		(μ = 29.8079550)		D ₀ ⁰ = 1.0 ₄ eV						JAN 1975 A
D (² Π _{3/2})	39703.5	341.8	H ^Q 1.87					D ↔ X, V	39727.7 H ^Q	(1)(3)* (9)* (13)*
C (² Π _{1/2})	(35782)	(383) ^a						C ↔ X, (V)	35828	(1)(2)(3)* (6)* (7)(8) (10)(12)(13)*
B ² Σ ⁺	23421.0	192.0 ^b	H 0.50 ^b					B → X, R _V	23371.0 H	(1)(2)(4)* (7)* (11)
X ² Σ ⁺	0	292.61	H 1.6025 ^c				[(2.23)] ^d			
(202) Hg ¹³³ Cs										
		(μ = 80.157999)		D _e = 0.050 eV ^a						JAN 1975 A
Diffuse V shaded absorption bands at 18710, 19140, 19560, 20270, 20750 cm ⁻¹ . Bands showing fine structure at 20030, 20060, 20090 cm ⁻¹ . Tentatively attributed to HgCs.										(1)
X ² Σ ⁺	0						5.0 ₉ ^a			(5)
(202) Hg ¹⁹ F										
		(μ = 17.3649660)		D ₀ ⁰ = (1.8) eV						JAN 1975
E	46770.6	587.6	H 10.1					E → X, ^a R	46818.4 H	(2)*
D (² Π _{3/2})	42999.6	469.4 ^b	H ^Q 10.05 ^b					D → X, V	42987.4 H ^Q	(1)*
C (² Π _{1/2})	(39044)	(506)	H					C → X, V	39053 H	(1)*
X ² Σ ⁺	0	490.8 ^c	H ^Q 4.05							

HgBr (continued):

- ^cFrom (12)(13). Earlier analyses of C-X by (4)(5) and (10) as well as the suggested existence of an additional system in the region 36100 - 37000 cm⁻¹ (10)(12) are not convincing.
- ^d $\omega_e \nu_e = -0.0090$.
- (1) Wieland, HPA 2, 46, 77 (1929).
 - (2) Wieland, ZP 77, 157 (1932).
 - (3) Wieland, HPA 12, 295 (1939).
 - (4) Sastry, CS 10, 197 (1941).
 - (5) Sastry, PNISI 7, 359 (1941).
 - (6) Howell, PRS A 182, 95 (1943).
 - (7) Rao, Rao, IJP 18, 281 (1944).
 - (8) Wieland, JCPFB 45, 3 (1948).
 - (9) Wieland, in "Contribution a l'Etude de la Structure Moléculaire", Vol. comm. Victor Henri, Ed. Desoer, Liège (1948), p. 229.
 - (10) Krishnamurthy, ZP 152, 242 (1958).
 - (11) Wieland, ZE 64, 761 (1960).
 - (12) Patel, Darji, IJP 42, 110 (1968).
 - (13) Greig, Gunning, Strausz, JCP 52, 3684 (1970).

- HgCl: ^aFrom the absorption spectrum (13).
- ^bFor $\nu \geq 30$: $\omega_e = 186.2$, $\omega_e x_e = 0.40$.
- ^c $\omega_e \nu_e = -0.01493$, $\omega_e z_e = -0.000033$. All constants refer to R heads of B-X. From Q heads of D-X $\omega_e = 293.4$, $\omega_e x_e = 1.82$.
- ^dFrom electron diffraction data (5); according to (7) more likely corresponding to the Hg-Cl separation in HgCl₂ than in HgCl.
- (1) See ref. (1) of HgBr.
 - (2) See ref. (2) of HgBr.
 - (3) Cornell, PR 54, 341 (1938).
 - (4) Wieland, ZPC B 42, 422 (1939).

HgCl (continued):

- (5) Maxwell, Mosley, PR 57, 21 (1940).
- (6) Sastry, PNISI 7, 351 (1941).
- (7) Wieland, HPA 14, 420 (1941).
- (8) See ref. (6) of HgBr.
- (9) Wieland, HCA 26, 1939 (1943).
- (10) See ref. (8) of HgBr.
- (11) See ref. (9) of HgBr.
- (12) Krishnamurthy, ZP 150, 287 (1958).
- (13) Horne, Gosavi, Strausz, JCP 48, 4758 (1968).

- HgCs: ^aFrom Cs-Hg scattering data (5); see also (2)(3)(4).
- (1) Barratt, TFS 25, 758 (1929).
 - (2) Morse, Bernstein, Hostettler, JCP 36, 1947 (1962).
 - (3) Morse, Bernstein, JCP 37, 2019 (1962).
 - (4) Neumann, Pauly, JCP 52, 2548 (1970).
 - (5) Buck, Kick, Pauly, JCP 56, 3391 (1972).

- HgF: ^aClose double heads.
- ^bAbove $\nu=4$: $\omega_e = 410$, $\omega_e x_e = 1.5$.
- ^cFrom D-X.
- (1) See ref. (6) of HgBr.
 - (2) Babu, Rao, Reddy, IJPAP 4, 467 (1966).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(202) Hg¹H										
		$(\mu = 1.00282118)$		$D_0^0 = 0.3744 \text{ eV}^a$						JAN 1976 A
D $2\Sigma^+$		Fragments only.		[(4.7)]			[(1.8 ₉)]	D→X, R (37040)		(2)(8)
C $2\Sigma^+$				[4.519] ^b		[34.8] ^c	[1.928 ₇]	C→X, R 35587.4 Z		(2)(8)(12)
B $2\Sigma^+$				[4.028] ^d		[16.27] ^e	[2.042 ₉]	B→X, ^f R 33876.47 Z		(1)(2)(8)(12)
A ₂ $2\Pi_{3/2}$	28274	2068.24 ^g Z	43.04 ^h	6.741 ₁ ^{gi}	0.2295 ^j	[2.818] ^{gk}	1.5791	A ₂ →X, ^l V 28616.23 ^m Z		(2)(4)(5)(6)(8)
A ₁ $2\Pi_{1/2}$		[1939.18] ^g Z	n	[6.5609] ^{gop}	q	[2.850] ^{gr}	[1.6007]	A ₁ →X, ^l V _R 24933.10 ^m Z		(2)(4)(5)* (6)(7)(8) (9)* (15)
X $2\Sigma^+$	0	[1203.24] ^g Z	s	[5.3888] ^{gptu}	v	[3.953] ^{gw}	[1.7662 ₀]	ESR sp. ^x Potential curve (14)(15).		
(202) Hg²H										
		$(\mu = 1.99421540)$		$D_0^0 = 0.3976 \text{ eV}^a$						JAN 1976
A $2\Pi_r$				[3.3342] ^{bc}		[0.724] ^b	[1.5923]	A→X, ^d V 26400.4 ^b		(1)(2)(3)(6)(7)
X $2\Sigma^+$	0	[896.12] Z	e	[2.738 ₅] ^{cfigh}	i	[0.91] ^{fj}	[1.7569]	ESR sp. ^k		
(202) Hg³H										
		$(\mu = 2.9716734_0)$		$D_0^0 = 0.4086 \text{ eV}^a$						JAN 1976
A ₁ $2\Pi_{1/2}$		[1150.8] H	^l					A ₁ →X, V 24776.1 H		(3)
X $2\Sigma^+$	0	[748.72] Z	m	[1.8464] ^{lno}	p	[0.4111] ^q	[1.7528]			

Hg¹H: ^aFrom the predissociation in X $2\Sigma^+$ of the hydride and deuteride (15). See also Fig. 189 of MOLSPEC, Vol. 1.
^bSpin doubling $\Delta v_{12} = + [2.71 - 0.0093 \times N(N+1)](N+\frac{1}{2})$, increasing rapidly above N=17. See also (13).
^cH₀ = + 3.42 × 10⁻⁶.
^dSpin doubling $\Delta v_{12} = + [1.11 - 0.00374 \times N(N+1)](N+\frac{1}{2})$, increasing very rapidly above N=19. See also (13).
^eH₀ = + 2.04 × 10⁻⁶.

Hg¹H (continued):

^fQ branches weak in 0-0, strong in 0-1 and 0-2, not observed in 0-3.
^gThese are effective constants; "true" vibronic energies and rotational constants calculated by (12).
^h $= 0.052_0(v+\frac{1}{2})^4$ [$v = 0, \dots, 6$].
ⁱPerturbations.

Hg¹H (continued):

- $j + 0.0083_9(v+\frac{1}{2})^2 - 0.0013_0(v+\frac{1}{2})^3$ [$v=0, \dots, 6$].
 $k_{D_1}, \dots, D_3(10^{-4}\text{cm}^{-1}) = 2.880, 2.867, 3.182$;
 $H_0, \dots, H_3(10^{-8}\text{cm}^{-1}) = +0.09, +0.07, -5.4, +2.46$.
 l_{Hg} "nuclear" isotope shifts; see (6).
 m Constants in (8) are slightly different since they refer to $J'=1/2$ or $3/2$ instead of $\{J'=0\}$ relative to $N''=0$.
 $n_{\Delta G(3/2, 5/2)} = 1809.66, 1509.13$.
 o Λ -type doubling $\Delta v_{fe}(v=0) = +3.360(J+\frac{1}{2}) - \dots$ (8); decreasing with increasing v , but very anomalous in $v=3$. See also (13).
 p Magnetic hyperfine structure in $X^2\Sigma^+$ and $A_1^2\Pi_{1/2}$ of $^{199}\text{Hg}^1\text{H}$ and $^{201}\text{Hg}^1\text{H}$, see (7)(9).
 $q_{B_1} = 6.3239, B_2 = 6.0271$ (perturbation by $v=0$ of A_2), $B_3 = 5.104$ (very anomalous, see r).
 $r_{D_1}, \dots, D_3(10^{-4}\text{cm}^{-1}) = 2.952, 3.462, -18.42$;
 $H_0, \dots, H_3(10^{-8}\text{cm}^{-1}) = +0.082, -1.21, -18.4, -31$.
 $s_{\Delta G(3/2, \dots, 7/2)} = 965.34, 632.53, 167.82, G(0) = 681.2$ (15).
 t Spin doubling $\Delta v_{12}(v=0) = +2.14_4(N+\frac{1}{2}) - \dots$; decreasing rapidly with increasing v (4)(9).
 u Predissociation by rotation. Lines with $N'' > 29, 22, 15$ in $v''=0, 1, 2$, resp., are broad. Lines with $N'' > 30, 24, 18, 8, 6$ in $v''=0, \dots, 4$, resp., are absent (3)(5)* (9).
 $v_{B_1}, \dots, B_4 = 4.9512, 4.3473, 3.2510, 1.451$.
 $w_{D_1}, \dots, D_4(10^{-4}\text{cm}^{-1}) = 5.016, 8.08, 33.87, 40.7$;
 $H_0, \dots, H_3(10^{-8}\text{cm}^{-1}) = -0.06, -4.99, -21.4, -1490$; high-
 x In solid Ar matrix at 4 K (11). | er order constants in (8).
 (1) Hulthén, ZP 50, 319 (1928).
 (2) Rydberg, ZP 73, 74 (1932).
 (3) Rydberg, ZP 80, 514 (1933).
 (4) Fujioka, Tanaka, Sci. Pap. IPCR (Tokyo) 34, 713 (1938).
 (5) Porter, JOSA 52, 1201 (1962).
 (6) Porter, Davis, JOSA 52, 1206 (1962).

Hg¹H (continued):

- (7) Porter, Davis, JOSA 52, 338 (1963).
 (8) Phillips, Davis, BAMS Vol. 2 (1968).
 (9) Eakin, Davis, JMS 35, 27 (1970).
 (10) Veseth, JP B 3, 1677 (1970).
 (11) Knight, Weltner, JCP 55, 2061 (1971).
 (12) Veseth, JMS 44, 251 (1972).
 (13) Veseth, JP B 6, 1484 (1973).
 (14) Kosman, Hinze, JMS 56, 93 (1975).
 (15) Stwalley, JCP 63, 3062 (1975).

Hg²H, Hg³H:

- a See a of Hg¹H.
 b "True" constants of (6) who gives doublet splitting and Λ -type doubling parameters. The heads of the 0-0 subbands are at 24810.6 and 28493.6 cm^{-1} .
 c Magnetic hfs in $X^2\Sigma^+(b=0.2010$ in $v=1)$ and $A^2\Pi_{1/2}$ of $^{199}\text{Hg}^2\text{H}$; see (3).
 d_{Hg} isotope effects (1). | of $^{199}\text{Hg}^2\text{H}$; see (3).
 $e_{\Delta G(3/2 \dots 11/2)} = 790.48, 660.35, 497.80, 264.92, 58.35, G(0) = 488.8$ (7).
 f Effective constants; "true" values for $v=0$ in (6).
 g Spin doubling $\Delta v_{12}(v=0) = +1.085(N+\frac{1}{2}) - \dots$; decreasing rapidly with increasing v .
 h Predissociation by rotation. Highest observed levels in $v=0 \dots 6$ are $N=43, 35, 31, 23, 15, 10, 8$ (3)(7).
 $i_{B_1 \dots 6} = 2.595_4, 2.422_5, 2.196_1, 1.845, 1.172_9, 0.732_5$.
 $j_{D_1 \dots 6}(10^{-4}\text{cm}^{-1}) = 1.14, 1.41, 2.02, 1.7, 16.27, (5.8)$.
 $H_0 \dots 5(10^{-8}\text{cm}^{-1}) = -0.9, -0.6_1, -1.7, -5.0, -110, -300$.
 k In solid argon at 4 K (5).
 l Magnetic hfs in $X^2\Sigma^+$ and $A_1^2\Pi_{1/2}$ of $^{199}\text{Hg}^3\text{H}$ (3).
 $m_{\Delta G(3/2 \dots 11/2)} = 680.34, 601.75, 509, 390, 240, G(0) = 402.6$ (7).
 (continued p. 319)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(202) Hg¹H⁺										
$D_0^0 = (2.9_9) \text{ eV}$										
A $1\Sigma^+$	44316.6	1623.6 ^a	Z 45.1 ₁ ^b	5.867 ^a	0.201 ^c	3.1 ^d	1.692 ₇	A→X, R	44112.6 Z	FEB 1975 (1)* (4)(5)
X $1\Sigma^+$	0	2027.7 ^a	Z 40.9	6.613	0.206	2.8 ₅	1.594 ₄			
(202) Hg²H⁺										
$D_0^0 = (3.0_1) \text{ eV}$										
A $1\Sigma^+$	44306.3	1151.2 ^a	Z 22.4 ₅ ^e	2.953	0.074 ^f	0.77 ^g	1.691 ₉	A→X, R	44161.9 Z	FEB 1975 (2)(3)(4)(5)
X $1\Sigma^+$	0	1438.5 ^a	Z 20.7	3.328	0.073 ₆	0.72	1.593 ₈			
(202) Hg⁴He										
$(\mu = 3.9248221_3)$ See ref. (1)(4)(5) of HgAr.										
(202) Hg¹²⁷I										
$(\mu = 77.935292_4) \quad D_0^0 = 0.35_4 \text{ eV}^a$										
H	47110	97.1	H 1.7	Predissociation above $v=2$.				H→X, R	47096 H	(2)(8)*
G	45542	88.4	H 0.2					G→X, R	45524 H	(2)(8)*
F ₃	(44531)	(85.5)	H (0.8)					F ₃ →X, R	(44510) H	(7)(9)
F ₂		Unclassified bands in the region 40800 - 42200 cm^{-1} , converging near 40800 cm^{-1} .						F ₂ →X, R		(7)(13)*
F ₁	40152	90.8	H 0.93					F ₁ →X, R	40135 H	(7)(9)
E		Bands in the region 37500 - 39500 cm^{-1} ; tentative analyses (4)(14).						E→X, R		(3)(4)(14)
D ($2\Pi_{3/2}$)	36269	178.0	H 1.14					D→X, V	36295 H	(3)(5)(6)
C ($2\Pi_{1/2}$)	32730.0	235.6	H 2.21					C↔X, V	32785.0 H	(1)(3)(5)(6) (10)(12)(16)
B $2\Sigma^+$	24187.1	110.45	H 0.15					B↔X, R	24180.0 H	(11)(15)*
X $2\Sigma^+$	0	125.0	H 1.0 ^b							

Hg²H, Hg³H (continued):

ⁿSpin doubling $\Delta v_{12}(v=0) = +0.744(N+\frac{1}{2}) - \dots$;

decreasing with increasing v.

^oPredissociation by rotation. The last observed levels in v=0,1,2 are N=51, 44, 39.

^pB₁, B₂, B₃ = 1.7691, 1.6806, 1.5757.

^qD₁, D₂, D₃ (10⁻⁴ cm⁻¹) = 0.4795, 0.5586, 0.7957;

H₀...H₃ (10⁻⁸ cm⁻¹) = -0.272, +0.057, -0.247, +1.66.

(1) Mrozowski, ZP 22, 236 (1936).

(2) See ref. (4) of Hg¹H.

(3) See ref. (9) of Hg¹H.

(4) See ref. (10) of Hg¹H.

(5) See ref. (11) of Hg¹H.

(6) See ref. (12) of Hg¹H.

(7) See ref. (15) of Hg¹H.

Hg¹H⁺, Hg²H⁺:

^aRe-evaluated from the data of (4).

^b $w_e y_e = -7.20$, calculated from the value for Hg²H⁺.

^c $y_e = -0.0455$.

^d $\beta_e = +0.4 \times 10^{-4}$.

^e $w_e y_e = -2.57$.

^f $y_e = -0.0105$.

^g $\beta_e = +0.10 \times 10^{-4}$.

(1) Hori, ZP 61, 481 (1930).

(2) Mrozowski, APP 4, 405 (1935).

(3) Hori, Huruti, ZP 101, 279 (1936).

(4) Mrozowski, Szulc, APP 6, 44 (1937).

(5) Mrozowski, PR 58, 332 (1940).

HgI: ^aExtrapolation for X ² Σ^+ (15). Good agreement with an earlier thermochemical value (12).

^bAbove v=7: $w_e x_e \approx 1.5$.

(1) See ref. (1) of HgBr.

(2) Prileshajewa, PZS 1, 189 (1932).

(3) Wieland, ZP 76, 801 (1932).

(4) Sastry, PNISI 8, 289 (1942).

(5) See ref. (6) of HgBr.

(6) Rao, Sastry, Krishnamurti, IJP 18, 323 (1944).

(7) Rao, Rao, IJP 20, 148 (1946).

(8) Ramasastry, Rao, IJP 21, 143 (1947).

(9) Ramasastry, IJP 22, 95 (1948).

(10) See ref. (8) of HgBr.

(11) See ref. (9) of HgBr.

(12) Wieland, Herczog, HCA 32, 889 (1949).

(13) Ramasastry, PNISI 18, 487 (1952).

(14) Krishnamurthi, ZP 160, 438 (1960).

(15) See ref. (11) of HgBr.

(16) Greig, Gunning, Strausz, JCP 52, 4569 (1970).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References	
								Design.	v_{00}		
$(202) \text{Hg}^{(115)} \text{In}$		$(\mu = 73.237853)$ Two diffuse emission bands extending to longer wavelengths from the In lines at 4511 Å (22160 cm ⁻¹) and 4102 Å (24373 cm ⁻¹). Fragments of a weak system of V shaded emission bands at 20020 cm ⁻¹ .								FEB 1975	
B	a + 19106	198	H					B → A, ^a	V 19130	H	(1) (1) (1)* (2)*
A	a	151	H								
$(202) \text{Hg}^{(39)} \text{K}$		$(\mu = 32.6625294)$ $D_e = 0.052 \text{ eV}^a$ Diffuse, V shaded absorption bands at 16160, 16260, 24310, 25070 cm ⁻¹ ; tentatively assigned to HgK.									FEB 1975 A
X	$2\Sigma^+$	0					4.9_1^a				(1) (5)
$(202) \text{Hg}^{(84)} \text{Kr}$		$(\mu = 59.281983_1)$ See ref. (1)(2)(5)(7)(10) of HgAr.									FEB 1975 A
$(202) \text{Hg}^{(7)} \text{Li}$		$(\mu = 6.7804667)$ $D_e = 0.105 \text{ eV}^a$									FEB 1975
X	$2\Sigma^+$	0					3.0_0^a				(2)(4)
$(202) \text{Hg}^{23} \text{Na}$		$(\mu = 20.640336_8)$ $D_e = 0.055 \text{ eV}^a$ Diffuse, V shaded absorption bands at 15380, 15490, 21510, 22590, 22690 cm ⁻¹ ; tentatively assigned to HgNa (1). Theoretical calculation of the lowest excited states (4).									SEP 1976 A
X	$2\Sigma^+$	0					4.7_2^a				(2)(3)
$(202) \text{Hg}^{(20)} \text{Ne}$		$(\mu = 18.1917011)$ See ref. (1)(5) of HgAr.									FEB 1975

HgIn: ^aDouble heads.

- (1) Purbrick, PR 81, 89 (1951).
- (2) Santaram, Winans, JMS 16, 309 (1965).

HgK: ^aFrom K-Hg scattering data (5); see also (2)(3)(4).

- (1)...(5) See ref. (1)...(5), resp., of HgCs.

HgLi: ^aFrom Li-Hg scattering data (2)(4); see also (1)(3).

- (1) Groblicki, Bernstein, JCP 42, 2295 (1965).
- (2) Olson, JCP 42, 4499 (1968).
- (3) See ref. (4) of HgCs.
- (4) Buck, Hoppe, Huiskens, Pauly, JCP 60, 4925 (1974).

HgNa: ^aFrom Na-Hg scattering data (2)(3).

- (1) See ref. (1) of HgCs.
- (2) See ref. (4) of HgCs.
- (3) Buck, Pauly, JCP 54, 1929 (1971).
- (4) Düren, CPL 39, 481 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$(202) \text{Hg}^{160} \text{O} ?$		$(\mu = 14.8211639_5)$ Absorption bands in the region $33900 - 36500 \text{ cm}^{-1}$, usually ascribed to Hg_2 ("wing" bands), were tentatively assigned to HgO by (1).							FEB 1975 (1)	
$(202) \text{Hg}^{(85)} \text{Rb}$ X $2\Sigma^+$ 0		$(\mu = 59.779505_9)$ $D_e = 0.049 \text{ eV}^a$ Diffuse, V shaded absorption bands at $15710, 15780, 20490 \text{ cm}^{-1}$ and other unclassified bands in the region $22700 - 23800 \text{ cm}^{-1}$; tentatively assigned to HgRb . 5.1 ^a							FEB 1975 A (1) (2)	
$(202) \text{Hg}^{(32)} \text{S}$		$(\mu = 27.6025696)$ $D_0^0 \leq 2.1_7 \text{ eV}^a$							FEB 1975	
$(202) \text{Hg}^{(80)} \text{Se}$		$(\mu = 57.259761_4)$ $D_0^0 \leq 1.6_9 \text{ eV}^a$							FEB 1975	
$(202) \text{Hg}^{(205)} \text{Tl}$		$(\mu = 101.730727)$ Four band systems in the red (15300 cm^{-1} , em. and abs.), green (19200 cm^{-1}), blue (22000 cm^{-1} , em.), and violet regions of the spectrum (26200 cm^{-1} , em. and abs.). Different vibrational analyses in (1) and (2), no details.							FEB 1975 A (1)(2)	
$(202) \text{Hg}^{(132)} \text{Xe}$		$(\mu = 79.792686_9)$ See ref. (1)(5)(10) of HgAr .							FEB 1975 A	

HgO: (1) Walter, Barratt, PRS A 122, 201 (1929).

HgRb: ^aFrom Rb-Hg scattering data (2).

(1) See ref. (1) of HgCs.

(2) See ref. (4) of HgCs.

HgS, HgSe:

^aThermochemical value (mass-spectrom.)(3)(4)(5).

Based on mass-spectroscopic evidence it is unlikely that three absorption continua with long-wavelength limits at 22500, 32200, 44400 cm^{-1} , observed by (1), and two absorption continua with long-wavelength limits at 22200, 38630 cm^{-1} , observed by (2), are due to HgS and HgSe, resp..

(1) Sen-Gupta, PRS A 143, 438 (1934).

(2) Mathur, IJP 11, 177 (1937).

(3) Colin, ICB 26, 1129 (1961).

(4) Goldfinger, Jeunehomme, TFS 52, 2851 (1963)

(5) Marquart, Berkowitz, JCP 32, 283 (1963).

HgTl: (1) Winans, Pearce, PR 74, 1262 (1948).

(2) Winans, Santaram, Pearce, Proc. Int. Conf. Spectrosc., Bombay (1967), Vol. I, p. 149.

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
[H¹²⁷]										
		$\mu = 0.99988453$ $D_0^0 = 3.054_1 \text{ eV}^a$ I.P. = 10.38 eV ^b								SEP 1976 A
L	[100640]	Broad absorption peak (width $\sim 4500 \text{ cm}^{-1}$). ^c						L \leftarrow X,	99500	(31)
H	(1) [75435]	First member of a Rydberg series converging to X $2\Pi_{1/2}(v=0)$ of HI^+ (I.P. = 11.05 eV); fragments of additional series. ^d						H \leftarrow X,	74290	(3)* (27)*
F	1Δ [71372.8]		[6.335] ^e		[2.3] ^e	[1.631]	F \leftarrow X,	R 70228.2	Z	(30)*
f ₁	$3\Delta_1$ [70831.5]		[6.015] ^f			[1.674]	f ₁ \leftarrow X,	R 69686.9	Z	(30)*
D	1Π [70389.0]		[6.198] ^g		[2.1] ^g	[1.649]	D \leftarrow X,	R 69244.4	Z	(30)*
d ₀	$3\Pi_0$ [70302.4]		[6.117] ^h		[2.1] ^h	[1.660]	d ₀ \leftarrow X,	R 69157.8 ^h	Z	(30)*
Additional unclassified absorption bands between 68100 and 69000 cm^{-1} .										
G	1 [70136.4]		[6.406] ⁱ		[3.2] ⁱ	[1.622]	G \leftarrow X,	(R) 68991.8	Z	(3)* (30)*
v	$1\Sigma^+$		[2.84] ^j		[2.0] ^j	[2.44] ^j	v \leftarrow X,	R 68004.4 ^j	Z	(30)*
E	$1\Sigma^+$ (66326)	[1681.8] Z		[6.110] k	[2.5] ^k	[1.661] ₁	E \leftarrow X,	R 66022.6	Z	(3)* (30)*
f ₂	$3\Delta_2$ [65838.6]		[6.757] ^l		[12.3] ^l	[1.580]	f ₂ \leftarrow X,	V 64694.0	Z	(30)*
f ₃	$3\Delta_3$ [65717.5]		[5.706] ^m		[-8.3] ^m	[1.719]	f ₃ \leftarrow X,	R 64572.9	Z	(30)*
e	$3\Sigma^+$ [65345]	Very diffuse feature.						e \leftarrow X,	64200	(30)*
d ₁	$3\Pi_1$ [65028]	Diffuse feature.						d ₁ \leftarrow X,	63883 H ^Q	(30)*
d ₂	$3\Pi_2$ (63922)	[2154.4] Z		[6.065] n	[1.7]	[1.667] ₃	d ₂ \leftarrow X,	R 63854.9	Z	(30)*
c	1Π (62378)	[2183] H ^Q	Diffuse, no rotational structure.					c \leftarrow X,	62325 H ^Q	(3)(20)
b ₀	$3\Pi_0$ { ⁰⁺ 60858.7 ⁰⁻ (60840)}	2314.7 ^o Z 54.3 ^o Diffuse Q head only.	6.493 ^o	0.118 ^o		1.611 ₄	b ₀ \leftarrow X,	60857.9 Z 60839 H ^Q	Z H ^Q	(20)* (30)* (20)*
b ₁	$3\Pi_1$ (56783)	[2200]		[6.427] (v=1 diffuse Q head)		[1.619] ₆	b ₁ \leftarrow X,	56738.3	Z	(3)(20)
b ₂	$3\Pi_2$ (55874)	[2207.4] Z		6.436	0.175	1.618 ₅	b ₂ \leftarrow X,	55833.1	Z	(20)*

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^1\text{H}^{127}\text{I}$ (continued)										
A ($^1\Pi$) a ($^3\Pi_0^+, ^3\Pi_1$) X $^1\Sigma^+$	0	Continuous absorption starting at ~ 28000 with maximum at $\sim 46000 \text{ cm}^{-1}$.					1.60916	A } \leftarrow X, p a }	(2)(4)(5) (17)(24)	
			2309.01 ₄	Z 39.643 ₅ ^q	[6.4263650] ^{rs}	0.1688 ₆ ^t		[2.069] ^r	Rot.-vibr. sp. ^u Rotation sp. ^{vw} Raman sp. ^x	(6)(12)(23) (26) (1)(7)(8)(22) (29)

¹HI: ^aFrom $D_0^0(\text{H}_2)$, $D_0^0(\text{I}_2)$, and $\Delta H_{f0}(\text{HI})$, from gaseous H_2 , I_2 .

^bFrom photoionization studies by (10); refers to $X^2\Pi_{3/2}$ of HI^+ . (18) give the same value, (15) give 10.42 eV from the photoelectron spectrum.

^cDiffuse on account of predissociation and preionization; presumably first member of a Rydberg series converging to A $^2\Sigma^+$ of HI^+ (31).

^dAbove the first ionization limit ($X^2\Pi_{3/2}$) the members of the series are subject to preionization and are seen as photoionization peaks (27).

^eAverage B and D, $B(2^+) - B(2^-) = -0.05$.

^fAverage B value, $B(1^+) - B(1^-) = +0.240$.

^gRefers to the 1^+ component; $B(1^-) \approx 6.25$.

^hConstants refer to the 0^+ component; for $0^- B_0 = 6.091$, $v_{00} = 69149.5$.

ⁱAverage B and D, $B(1^+) - B(1^-) = +0.107$.

^jVibrational numbering uncertain; the numbers given refer to the lowest level observed in absorption for which v is probably fairly high. Several higher vibrational levels have been found; strong perturbations.

^k $B_1 = 5.62$, $D_1 = 28 \times 10^{-4}$, perturbed at high J.

^lAverage B and D, $B(2^+) - B(2^-) = -0.040$.

^mAverage B and D, $B(3^+) - B(3^-) = +0.018$.

ⁿ $B_1(^3\Pi_2) = 5.92_3$.

^oFrom $v=0,1,3$ only; $\gamma_e = -0.031_7$.

^pPhotofragment spectroscopy at 37550 cm^{-1} (28) shows that the continuum is of composite nature; 36% of the absorption is due to $^3\Pi_0^+$ yielding $\text{H} + \text{I}(^2P_{1/2})$. (28) have analysed the continuum in terms of three overlapping transitions $^1\Pi$, $^3\Pi_0^+$, $^3\Pi_1 \leftarrow$ X. A very weak continuum with maximum at 23500 cm^{-1} was reported by (4).

^q $\omega_e y_e = -0.0200$, $\omega_e z_e = +0.01621$, from the 1-0,...,4-0 vibr.-rot. bands (23); very slightly different constants are given by (26) who have measured the 5-0 and 6-0 bands.

^rMicrowave value (22).

^sDunham potential coefficients (32).

^t $\gamma_e = -0.00095$; from (23), see ^q.

^uThe 1-0,...,6-0 bands have been observed in absorption. Ab-

(continued on p. 327)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
2H ¹²⁷ I											
		$\mu = 1.98263579$	$D_0^0 = 3.094_9 \text{ eV}^a$						SEP 1976 A		
F $^1\Delta$	[71069.9]			[3.161]		[0.51]	[1.640]	F \leftarrow X, R	70255.0 Z	(9)	
Further unclassified absorption bands between 68100 and 69800 cm^{-1} .											
f ₁ $^3\Delta_1$	[70513.3]			[3.089] ^b		[0.45] ^b	[1.659]	f ₁ \leftarrow X, R	69698.4 Z	(9)*	
D $^1\Pi$	[70065.5]			[3.155] ^c		[0.55] ^c	[1.642]	D \leftarrow X, R	69250.6 Z	(9)*	
d ₀ $^3\Pi_0$	[69972.1]			[3.131] ^d		[0.47] ^d	[1.648]	d ₀ \leftarrow X, R	69157.2 ^d Z	(9)*	
v $^1\Sigma^+$				[1.30] ^e			[2.56] ^e	V \leftarrow X, R	67893.6 ^e Z	(9)	
E $^1\Sigma^+$	66163.5	1455.9	Z 75.9 ₅	[3.092]	f	[0.60]	[1.658]	E \leftarrow X, R	66057.6 Z	(9)*	
f ₂ $^3\Delta_2$	[65533.6]			[3.296] ^g		[1.64] ^g	[1.606]	f ₂ \leftarrow X, R	64718.7 Z	(9)	
f ₃ $^3\Delta_3$	[65440.7]			[3.002] ^g		[0.22] ^g	[1.68 ₃]	f ₃ \leftarrow X, R	64625.8 Z	(9)	
e $^3\Sigma^+$	[65095]	Very diffuse feature.						e \leftarrow X, R	64280	(9)	
d ₁ $^3\Pi_1$	(63958)	[(1586)] ^h		[3.135] ^g		[0.39] ^g	[1.647]	d ₁ \leftarrow X, R	63936.2 Z	(9)	
d ₂ $^3\Pi_2$	[64681.5]			[3.111]		[0.39]	[1.653]	d ₂ \leftarrow X, R	63866.6 Z	(9)	
C $^1\Pi$	62321	1664	30	Diffuse Q heads only.				C \leftarrow X, R	62331 H ^Q	(5)	
b ₀ $^3\Pi_0$ 0^+	[61667.4]			[3.255]			[1.616]	b ₀ \leftarrow X, R	60852.5 Z	(5)*	
	[61647]			Diffuse, unresolved Q branch.					60832 H		
b ₁ $^3\Pi_1$	[57547.6]			[3.245] ⁱ			[1.619]	b ₁ \leftarrow X, R	56732.8 Z	(5)*	
b ₂ $^3\Pi_2$	(55862)	[1585.2]	Z	3.265 ₁	0.063 ₂		1.613 ₇	b ₂ \leftarrow X, R	55840.1 Z	(5)*	
A ($^1\Pi$)	}	Continuous absorption starting at 33000 with maximum at 45000 cm^{-1} .									
a ($^3\Pi$)									A } \leftarrow X, j		(8)
x $^1\Sigma^+$	0	1639.65 ₅	Z 19.87 ₃ ^k	[3.2534872] ^l	0.06082 ^k	[0.5264] ^l	1.60909	Rot.-vibr. sp.		(2)(7)	
									Rotation sp. ^m		(1)(3)(4)(6)

²HI: ^aFrom $D_0^0(1\text{HI})$.

^bAverage B and D, $B(1^+) - B(1^-) = + 0.064$.

^cAverage B and D, $B(1^+) - B(1^-) = - 0.014$.

^dThe constants refer to the 0^+ component; the numbering of the Q branch (0^- component, $\nu_{00} \approx 69147.0$) is uncertain.

^eSee j of 1HI .

^f $B_1 = 2.97_4$ (perturbed at intermediate J), $B_2 = 2.80_2$.

^gConstants refer to the Ω^+ component.

^hThe 1-0 band is quite diffuse and its assignment uncertain.

ⁱBroad P and R lines, diffuse and unresolved Q branch.

²HI (continued):

^jAt 37550 cm⁻¹ 26% of the absorption is due to ³Π₀⁺; see P
^k_wy_e = -0.045₉, γ_e = -0.00017₆ from the IR sp. (7). | of ¹HI.
^lMicrowave value (6).
^mμ_{el}(v=0) = 0.31₆ D (3). Iodine hfs constants in (6).

(1) See ref. (7) of ¹HI.

(2) Jones, JMS 1, 179 (1957).

(3) Burrus, JCP 28, 427 (1958).

(4) Cowan, Gordy, PR 111, 209 (1958).

(5) See ref. (20) of ¹HI.

(6) See ref. (22) of ¹HI.

(7) See ref. (23) of ¹HI.

(8) See ref. (24) of ¹HI.

(9) See ref. (30) of ¹HI.

¹HI (continued):

solute intensities, dipole moment function (9)(11)(14)(16)
 (25). The R branch of the fundamental is much stronger
 than the P branch on account of rotation-vibration inter-
 action; for the overtones this effect is very small (11)
 (14). The overall intensities decrease rather slowly in
 the series 1-0, 2-0, 3-0 (11)(14). Line width, pressure
 broadening studied by (9)(14).

^vFrom the hfs of the microwave spectrum (19) derive nuclear
 quadrupole (I) and other hyperfine coupling constants; see
 also (22). From the Stark effect in the hfs of the 1-0
 transition (21) obtain μ_{el}(v=0) = 0.4477 D.

^wAbsolute intensities (13).

^xVibrational Raman cross sections.

(1) Czerny, ZP 44, 235 (1927).

(2) Goodeve, Taylor, PRS A 154, 181 (1936).

(3) Price, PRS A 167, 216 (1938).

(4) Datta, Kundu, PNISI 7, 311 (1941).

(5) Romand, AP(Paris) (12) 4, 529 (1949).

(6) Boyd, Thompson, SA 5, 308 (1952).

(7) Palik, JCP 23, 217 (1955).

(8) Cowan, Gordy, PR 104, 551 (1956).

(9) Ameer, Benesch, JCP 37, 2699 (1962).

(10) Watanabe, Nakayama, Mottl, JQSRT 2, 369 (1962).

(11) Benesch, JCP 39, 1048 (1963); 40, 422 (1964).

(12) Haeusler, Meyer, Barchewitz, JP(Paris) 25, 961 (1964).

(13) Chamberlain, Gebbie, Nature 208, 480 (1965).

(14) Meyer, Haeusler, Barchewitz, JP(Paris) 26, 305 (1965).

(15) Frost, McDowell, Vroom, JCP 46, 4255 (1967).

(16) Jacobi, JMS 22, 76 (1967).

(17) Huebert, Martin, JPC 72, 3046 (1968).

(18) Lempka, Passmore, Price, PRS A 304, 53 (1968).

(19) Van Dijk, Dymanus, CPL 2, 235 (1968).

(20) Tilford, Ginter, Bass, JMS 34, 327 (1970).

(21) Van Dijk, Dymanus, CPL 5, 387 (1970).

(22) De Lucia, Helminger, Gordy, PR A 3, 1849 (1971).

(23) Hurlock, Alexander, Rao, Dreska, JMS 37, 373 (1971).

(24) Ogilvie, TFS 67, 2205 (1971).

(25) Tipping, Forbes, JMS 32, 65 (1971).

(26) Bernage, Niay, Houdart, CR B 278, 235 (1974).

(27) Tsai, Baer, JCP 61, 2047 (1974).

(28) Clear, Riley, Wilson, JCP 63, 1340 (1975).

(29) Cherlow, Hyatt, Porto, JCP 63, 3996 (1975).

(30) Ginter, Tilford, Bass, JMS 57, 271 (1975).

(31) Terwilliger, Smith, JCP 63, 1008 (1975).

(32) Ogilvie, Koo, JMS 61, 332 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References			
								Design.	v_{00}				
$^3\text{HI}^{127}\text{I}$ X $1\Sigma^+$ 0		$\mu = 2.9460334_1$					[2.193261]	[2.385] ^a	[1.615230]	Microwave sp. ^b	SEP 1976 (1)(2)		
$^1\text{HI}^{127}\text{I}^+$ A $2\Sigma^+$ (28000) ^c X $2\Pi_{1/2}$ (5400) ^c $2\Pi_{3/2}$ 0		d	$D_0^0 = 3.12_5 \text{ eV}^a$ I.P. = 19.6 eV^b							(1.62) ^e	SEP 1976		
$^1\text{HI}^{127}\text{I}^-$		Resonances due to inverse preionization have been found in the electron transmission current in the range 6.7 - 10.0 eV. They correspond to excited states of HI^- in which two electrons are in Rydberg orbitals $ns6^2$, $np6^2$, or $nd\lambda^2$ while the core is in the X $2\Pi_{3/2}$ or $2\Pi_{1/2}$ state of HI^+ .									(1)	SEP 1976	
$^{165}\text{Ho}_2$		$\mu = 82.465179$					$D_0^0 = 0.8_2 \text{ eV}^a$					FEB 1975	
$^{165}\text{Ho}^{19}\text{F}$ B 21240.9 A 19152.77 X d 0		502.2 H 2.9 539.45 Z 4.3 ₉ 615.28 Z 2.60 ₃	$D_0^0 = 5.5_7 \text{ eV}^a$					0.24591 ^c 0.26295	0.00217 0.00145	[0.0173] [0.0178]	2.0060 1.9399	B \leftarrow X, ^b R 21184.2 H (2) A \leftarrow X, ^b R 19114.41 Z (2)*	
$^{165}\text{Ho}^{16}\text{O}$		$\mu = 14.5808654_3$					$D_0^0 = 6.3_9 \text{ eV}^a$	R shaded emission bands from 21700 to 23000 cm^{-1} . Two complicated groups of R and V shaded emission bands in the regions 16900 - 18000 and 18500 - 19800 cm^{-1} .				(18795) (17881)	FEB 1975 A (3) (1)* (2)*

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{165}\text{Ho}^{(32)}\text{S}$		$(\mu = 26.7806009)$		$D_0^0 = 4.3_8 \text{ eV}^a$						FEB 1975
$^{165}\text{Ho}^{(80)}\text{Se}$		$(\mu = 53.832260_1)$		$D_0^0 = 3.4_1 \text{ eV}^a$						FEB 1975

^3HI : ^aCalculated by isotope relations from HI and DI (2).

^bIodine hyperfine structure constants.

(1) Rosenblum, Nethercot, PR 27, 84 (1955).

(2) De Lucia, Helming, Gordy, PR A 3, 1849 (1971).

$^1\text{HI}^+$: ^aFrom $D_0^0(\text{HI}) + \text{I.P.}(\text{I}) - \text{I.P.}(\text{HI})$.

^bFrom the electron impact appearance potential of HI^{++} (1).

^cFrom the photoelectron spectrum (2)(3).

^dUnlike those of HF, HCl, HBr, the $A^2\Sigma$ photoelectron peak of HI is very broad and without vibrational structure, clearly suggesting that the $A^2\Sigma^+$ state of HI^+ is strongly predissociated. (3) estimate $\Delta G(\frac{1}{2}) \approx 1040$, $r_e \approx 1.90$.

^eEstimated by (3) from the constants for HF^+ , HCl^+ , HBr^+ .

(1) Dorman, Morrison, JCP 35, 575 (1961).

(2) Frost, McDowell, Vroom, JCP 46, 4255 (1967).

(3) Lempka, Passmore, Price, PRS A 304, 53 (1968).

$^1\text{HI}^-$: (1) Spence, Noguchi, JCP 63, 505 (1975).

Ho_2 : ^aThermochemical value (mass-spectrom.)(1).

(1) Cocke, Gingerich, JPC 75, 3264 (1971).

HoF : ^aThermochemical value (1).

^bP, Q, and R branches.

^cPerturbations.

^dPossibly lowest component of an inverted triplet or quintet state with large spin-orbit splitting.

(1) Zmbov, Margrave, JPC 70, 3379 (1966).

(2) Robbins, Barrow, JP B 7, L234 (1974).

HoO : ^aThermochemical value (mass-spectrom.)(4), recalc. (5).

(1) Gatterer, RS 1, 139 (1942).

(2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(3) Mavrodineanu, Boiteux, "Flame Spectroscopy", Wiley (1965).

(4) Ames, Walsh, White, JPC 71, 2707 (1967).

(5) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

HoS : ^aThermochemical value (mass-spectrom.)(1), recalc. (2).

(1) See ref. (5) of HoO .

(2) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

HoSe : ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (2) of HoS .

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	ν ₀₀	
¹²⁷ I ₂		μ = 63.452237 ₈ D ₀ ⁰ = 1.54238 eV ^a I.P. = (9.311) eV ^b							JAN 1977 A	
		The absorption spectrum from 450000 to 870000 cm ⁻¹ (55.8 to 107.9 eV) at low resolution has been described by (55). It corresponds to excitation from the 4d shell to various unfilled orbitals.							(55)	
		The absorption spectrum in the VUV region at high resolution has most recently been photographed by (27) who gives an extensive table of observed features in the region 56500 - 75800 cm ⁻¹ . Most of the bands are assigned to extended Rydberg series converging to a common limit at 75814 cm ⁻¹ (9.400 eV), a smaller number to fragments of series converging to 80895 cm ⁻¹ (10.03 eV). The limits are assumed to correspond to ν=0 of X ² Π _g , ³ / ₂ and ¹ / ₂ , respectively, of I ₂ ⁺ ; see, however, ^b . Several of the progressions observed in absorption (27) appear to correspond to emission bands recorded by (11) under medium resolution in the region 56000 - 68000 cm ⁻¹ and classified by them as belonging to twelve systems. See also (6)(25)*.							(11)(27)*	
I	(51973) ^c	112.4	H	0.70 ₅ ^d				I → (B), ^c R	36197	H (9)(12)(32)
(H)	(46063)	103.7	H	0.09 ₅				(H → B), ^e R	30283	H (12)(32)
F (¹ Σ _u ⁺)	^f 47217.8	95.95 ₅	H	0.3623			(3.6) ^g	F ↔ X, ^h R	47158.6	H (12)(32)(47)*
F'	45230	93.4	H	0.6				F' → X, ⁱ R	45169	H (11)
G' (³ Π _{1g})	^j (42300)	{ Suggested upper state of high temperature absorption "continuum" shortward of 3263 Å (30640 cm ⁻¹).						G' ← A,		(5)(32)
E ³ Π _{0g} ⁺	^j 41411.4	101.59	H	0.238 ₀			(3.65)	E → B, ^k R	25630.5	H (13)(32)(47)*
D ¹ Σ _u ⁺	^l (40679)	104.41	H	0.243 ^m				D ↔ X, ⁿ R	(40624)	(25)* (32) (36)
G ³ Π _{2g}	^j (40300)	{ Suggested upper state of high temperature absorption "continuum" shortward of 3427 Å (29170 cm ⁻¹).						G ← A', ^o		(5)(32)
C ³ Σ _{lu} ⁺	^l	{ Repulsive state from ² P _{3/2} + ² P _{1/2} responsible for a weak but broad absorption continuum with maximum at 2700 Å (37000 cm ⁻¹). ^p						C ← X		(7)(10)(32)

- I_2 : ^aFrom the convergence of the vibrational levels in the B $^3\Pi_{0+u}$ state (49)(50).
^bFrom the photoelectron spectrum (33)(56); adiabatic potential established by temperature variation. The same method yields 9.953 eV for the ionization potential to $^2\Pi_{1/2g}(v=0)$. Neither result agrees with the values obtained by (27) from Rydberg series, i.e. 9.400 and 10.03 eV. The discrepancy could be understood if the Rydberg series were to correspond to $v'=3$, but the absence of series with $v'=0,1,2$ would still be puzzling.
^cWeak emission bands in the presence of foreign gases, 2785 - 2731 Å. T_e is based on the assumption that the lower state is the B state, but (36) has suggested that instead it may be the D state leading to $T_e \approx 76872 \text{ cm}^{-1}$.
^d $w_e y_e = +0.004$.
^eStrong emission bands in the presence of foreign gases, 3460 - 3015 Å. It is by no means certain that the lower state has been correctly identified as the B state. (35) suggests that the bands arise from the transition $G \rightarrow A'$.
^fConfiguration ... $6_g^2 \pi_u^3 \pi_g^3 6_u^2$.
^gFrom the intensity distribution and Franck-Condon principle (32)(47).
^hIn emission in electric discharges in the presence of foreign gases, 2740 - 2490 Å. Also observed for $^{129}I_2$, confirming the vibrational numbering. Emission bands in the region 2240 - 1950 Å are assigned by (11) to a separate system (called H \rightarrow X) with $v_{00} = 48072$ and $\omega \approx 79$. It seems, however, possible that these bands belong to F \rightarrow X.
ⁱThe analysis of this fairly extensive system [2400 - 2240 Å, called E \rightarrow X by (11)] is not yet supported by isotope studies, nor is it seen in absorption.
^jConfiguration ... $6_g \pi_u^4 \pi_g^3 6_u^2$.
^kEmission bands in the presence of foreign gases, 4400 -

4000 Å. Also observed for $^{129}I_2$, confirming the vibrational numbering. The E \rightarrow B fluorescence spectrum following two-photon absorption (77) consists of transitions both to the discrete and to the continuous part of B, the latter giving rise to diffuse bands ("structured" continuum)(83). From a comparison of the calculated with the observed intensity distribution (83) obtains the potential function of E as well as the variation of the transition moment with r . The lifetime of E \rightarrow B is 27 ns (82) confirming that this is an allowed transition and that the E state is $^3\Pi_{0+g}$.

^lConfiguration ... $6_g \pi_u^4 \pi_g^4 6_u$.

^m $w_e y_e = +0.00045$; the v' numbering is uncertain and, therefore, the vibrational constants are subject to change.

ⁿThe system includes the absorption bands of (2)(3)(6), remeasured by (20). It also includes the resonance series of (14) in the region 1830 - 2370 Å which arise from very high vibrational levels ($v' \approx 195$) of the D state excited by the 1830 Å atomic line of iodine. The system further includes the diffuse emission bands in the region 2500 - 5000 Å with a characteristic group near 3250 Å [McLennan bands (1)]. The diffuse bands have been recognized by (32) to correspond to transitions from D to the continuum of X [Condon diffraction bands, see also (72)]. Earlier summaries (10) (11)(27) gave an electronic state at $T_e = 51427.9$ with $w_e = 169.41$, $w_e x_e = 0.941$, $w_e y_e = +0.0022$ which was to represent the Cordes absorption bands from 1950 to 1795 Å (6). Following (32)(36) we consider these bands as part of D \leftarrow X.

^oThe G \rightarrow A' transition has been observed to lase strongly when mixtures of HI or CF₃I or CH₃I with argon (1000 - 4000 torr) are excited by a pulsed high current electron beam (89). See also H \rightarrow B, footnote ^e.

^pNature of the upper state (1_u) and of the dissociation products confirmed by photofragment spectroscopy (54).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-9} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
¹²⁷ I ₂ (continued)										
B'' ¹ Π_{1u} q		{Repulsive state from ² P _{3/2} + ² P _{3/2} , responsible for absorption continuum with maximum at 20050 cm ⁻¹ and for the predissociation of B ³ Π_{0+u} .						B'' \leftrightarrow X, r	(31)(60)(73)	
B' ³ Π_{0-u} q		{Repulsive state from ² P _{3/2} + ² P _{3/2} . The previous assignment of B' as the state responsible for the magnetic field induced predissociation of B is now in doubt; see ^u .								
B ³ Π_{0+u} q	15769.01	125.69 ₇	Z 0.764 ₂ st	0.02903 ₉ ^{uv}	0.000158 ₂ ^{wt}	5.4 ₃ ^x	3.024 ₇	B \leftrightarrow X, ^{ryz} R 15724.57 ^a Z	(50)(59)* (70)	
A ³ Π_{1u} q (11888)		(44.0) ^b	H (1.0)	b'				A \leftarrow X, ^c R (11803) ^b	(4)(60)	
A' ³ Π_{2u} q (10100)		Suggested as lower state of high temperature absorption bands near 3427 \AA (32)(35).								
X ¹ Σ_g^+ 0	0	214.50 ₂ ^d	Z 0.614 ₇ ^d	0.03737 ₂ ^{d'g}	0.000113 ₈ ^d	4.2 ₅ ^e	2.666 ₃	Raman sp. ^f	(48)(71)	

I₂ (continued):

^qConfiguration ... $\sigma_g^2 \pi_u^4 \pi_g^3 \sigma_u^-$.

^r_f values based on magnetic circular dichroism spectra have been estimated as 0.0018 (B'' \leftarrow X) and 0.009 (B \leftarrow X) and have been compared with earlier results (78). For a comparison of theoretical and observed intensities in the B \rightarrow X resonance series see (17).

^s - 0.00178($v + \frac{1}{2}$)³ - 0.0000738($v + \frac{1}{2}$)⁴ + 0.00000103($v + \frac{1}{2}$)⁵, from levels with $4 \leq v \leq 50$ (50).

^tSomewhat different constants, valid for $4 \leq v \leq 77$, are given by (70): $T_e = 15768.32$, $w_e = 126.165$, $w_e x_e = 0.8673$, ..., $B_e = 0.028939$, $\alpha_e = 0.0001204$, ... (using calculated D_v values); see also (51)(90). RKR potential curve (50). For a discussion of the long-range potential and ΔG , B_v values near the dissociation limit see (29)(39)(50)(58)(62)(66).

^uCollision induced predissociation of the B state (21); magnetic field induced predissociation (22)(42)(43); spontaneous predissociation (46); hyperfine predissociation (86). The purely radiative lifetime (37)(46)(86) increases smoothly from 0.91 μs at $v=7$ to approximately 10 μs at the highest observed levels. The measured lifetimes (37)(41)(52)(57)(76)(80) are considerably reduced by spontaneous predissociation due to rotational and hyperfine mixing with B'' ¹ Π_{1u} , the latter leading to differences in lifetime between ortho and para levels (86). Only near $v=12$ and above $v \approx 50$ are the actual lifetimes close to the purely radiative ones. The magnetic field induced predissociation of B ³ Π_{0+u} was previously assumed to be caused by B' ³ Π_{0-u} , and a potential function for this latter state was derived

I_2 (continued):

from magnetic quenching data (43)(53). The recent observation, however, of a quantum interference effect between magnetic and spontaneous predissociations (64)(68)(85) has established that the magnetic predissociation, too, is produced by the $B''^1\Pi_{lu}$ state.

$^v g_J$ varies from -0.059 at low v to $-5.45 \mu_N$ near the dissociation limit; from Hanle effect observations (38)(79)(87)(88). See also (69).

$w = 3.36 \times 10^{-7}(v+\frac{1}{2})^2 - 4.78 \times 10^{-8}(v+\frac{1}{2})^3 + 3.26 \times 10^{-10}(v+\frac{1}{2})^4$, from levels with $4 \leq v \leq 77$ (50).

$^x \beta_e \approx +0.30 \times 10^{-9}$ for $v \leq 10$ (50). D_v increases rapidly above $v=20$; for more details see (51)(70).

y The continuum joining onto the discrete bands is overlapped by the $B'' \leftarrow X$ continuum. A resolution of these two continua and the $A \leftarrow X$ continuum was given by (60). See also (61).

z The hyperfine structure of several lines has been observed by various high resolution laser techniques; electric quadrupole, magnetic octupole, and other magnetic hfs constants have been evaluated (23)(24)(28)(30)(34)(40)(45)(63)((65)(74)(81); similar analyses for $^{129}I_2$ and $^{127,129}I_2$ (84).

a Extrapolated from data with $v' \geq 4$. The vibrational numbering, changed (19) by 1 from the previous table in *MOLSPEC 1*, has been confirmed by isotope studies (18).

b (60) suggests that the v' numbering of (4) may have to be raised substantially. Preliminary results of a rotational analysis (92) of nine bands in the $A \leftarrow X$, $v''=5$ progression and of three bands in the $v''=4$ progression indicate that $w' \approx 57.5$, $w'x' \approx 1.85$, B' (for the lowest analyzed level) $= 0.02375$, $\alpha' \approx 0.0005$.

c The continuum joining onto the discrete bands has been studied by many investigators, most recently by (60) who derives an f value of 0.00062; see also (78).

d These constants (50) represent the levels $v=0-5$; (70), for $v=0-6$, give $w_e = 214,582$, $w_e x_e = 0.6243$, $B_e = 0.037363$, $\alpha_e = 0.0001145$ using calculated D_v values. On the basis of the resonance series of (8)(16) and (14), (26) has given polynomial formulae for $G(v)$, B_v , and D_v valid up to $v=82$: $w_e = 214.548$, $w_e x_e = 0.6163$, ..., $B_e = 0.037395$, $\alpha_e = 0.0001244$, ..., $D_e = 4.54 \times 10^{-9}$, $\beta_e = 0.017 \times 10^{-9}$, The most accurate constants for $v=0$ were derived (91) from the analysis by means of Fourier transform spectroscopy of the $B \leftarrow X$, 30-0 band: $B_0 = 0.0373115$, $D_0 = 4.55 \times 10^{-9}$, $H_0 = -0.76 \times 10^{-15}$.

The vibrational levels of the ground state have been observed up to $v=84$ [$D \rightarrow X$ resonance series (14)], i.e. to within 400 cm^{-1} of the dissociation limit. The levels $v'' = 98...115$ originally reported by (14) were found to be due to an NO impurity (67). As a consequence the RKR potential function of (14) must be corrected at high v . The RKR curves of (17) and (26) extend only to $v=82$ and are unaffected by this correction.

e $\beta_e = +0.32 \times 10^{-9}$; see d .

f High resolution resonance Raman spectra of I_2 vapour up to the eleventh overtone (12-0). Raman spectra in rare gas matrices (75).

g $g_J(v=0, J=12,14) = 9.13 \times 10^{-4} \mu_N$ from non-linear level crossing (44).

References on p.335 and 337.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{127}\text{I}_2^+$		$\mu = 63.452101$ $D_0^0 = (2.683) \text{ eV}^a$							JAN 1977	
B ($^2\Sigma_g^+$)	(27900) ^b									
A ($^2\Pi_{\frac{1}{2}u}$)	(18950) ^b									
A ($^2\Pi_{\frac{3}{2}u}$)	(12420) ^b									
X ($^2\Pi_{\frac{1}{2}g}$)	5180 ^c	220 ^d								
X ($^2\Pi_{\frac{3}{2}g}$)	0	240 ^d								
$^{127}\text{I}_2^-$		$\mu = 63.452375$ $D_0^0 = 1.04 \text{ eV}^a$ I.P. = 2.56 eV ^b							JAN 1977	
E ($^2\Pi_{\frac{1}{2}g}$)	(72100)	Resonances (due to inverse preionization) in the electron transmission current at 5.78 and 6.38 eV. ^c							(3)	
E ($^2\Pi_{\frac{3}{2}g}$)	(67300)									
X ($^2\Sigma_u^+$)	0									

I_2^+ : ^aFrom $D_0^0(\text{I}_2) + \text{I.P.}(\text{I}) - \text{I.P.}(\text{I}_2)$; the uncertainty in the ionization potential of I_2 (see ^b of I_2) makes $D_0^0(\text{I}_2^+)$ equally uncertain.
^bFrom photoelectron spectra (1)(4).
^cFrom the photoelectron spectrum (5). (1) obtain 5080.
^dAverage vibrational spacings in the photoelectron spectrum of (5). Good agreement for the $\frac{3}{2}$ component with $w = 238$ from the resonance Raman spectrum in solution (2).
 (1) Frost, McDowell, Vroom, JCP 46, 4255 (1967).
 (2) Gillespie, Morton, JMS 30, 178 (1969).
 (3) See ref. (27) of I_2 .
 (4) Cornford, Frost, McDowell, Ragle, Stenhouse, JCP 54,
 (5) See ref. (56) of I_2 . | 2651 (1971).

I_2^- : ^aFrom $D_0^0(\text{I}_2)$ and the electron affinities of I and I_2 .
^bFrom endoergic charge transfer, weighted average of the values in (1) and (2).
^cThe $^2\Pi_{ig}$ excited state is derived from the "grandparent" $X^2\Pi_{ig}$ of I_2^+ by the addition of a pair of ns σ Rydberg electrons. Weaker resonances at 6.85 and 7.15 eV may be associated with the configuration ...ns σ np σ /w.
 (1) Chupka, Berkowitz, Gutman, JCP 55, 2724 (1971).
 (2) Baede, Physica 52, 541 (1972).
 (3) Spence, PR A 10, 1045 (1974).

I₂ (continued):

- (1) McLennan, PRS A 88, 289 (1913); 91, 23 (1914).
- (2) Pringsheim, Rosen, ZP 50, 1 (1928).
- (3) Kimura, Miyanishi, Sci. Pap. IPCR (Tokyo) 10, 33 (1929).
- (4) Brown, PR 38, 1187 (1931).
- (5) Skorko, Nature 131, 366 (1933); APP 3, 191 (1934).
- (6) Cordes, ZP 97, 603 (1935).
- (7) Kortüm, Friedheim, ZN 2 a, 20 (1947).
- (8) Rank, Baldwin, JCP 19, 1210 (1951).
- (9) Venkateswarlu, PR 81, 821 (1951).
- (10) Mathieson, Rees, JCP 25, 753 (1956).
- (11) Haranath, Rao, JMS 2, 428 (1958).
- (12) Verma, PIAS A 48, 197 (1958).
- (13) Haranath, Rao, IJP 34, 123 (1960).
- (14) Verma, JCP 32, 738 (1960).
- (15) Weissman, Vanderslice, Battino, JCP 39, 2226 (1963).
- (16) Rank, Rao, JMS 13, 34 (1964).
- (17) Zare, JCP 40, 1934 (1964).
- (18) Brown, James, JCP 42, 33 (1965).
- (19) Steinfeld, Zare, Jones, Lesk, Klemperer, JCP 42, 25 (1965).
- (20) Nobs, Wieland, HPA 39, 564 (1966).
- (21) Steinfeld, JCP 44, 2740 (1966).
- (22) Degenkolb, Steinfeld, Wasserman, Klemperer, JCP 51, 615 (1969).
- (23) Hanes, Dahlstrom, APL 14, 362 (1969).
- (24) Kroll, PRL 23, 631 (1969).
- (25) Myer, Samson, JCP 52, 716 (1970).
- (26) Le Roy, JCP 52, 2683 (1970).
- (27) Venkateswarlu, CJP 48, 1055 (1970).
- (28) Hänsch, Levenson, Schawlow, PRL 26, 946 (1971).
- (29) Le Roy, Bernstein, JMS 37, 109 (1971).
- (30) Hanes, Lapierre, Bunker, Shotton, JMS 39, 506 (1971).
- (31) Oldman, Sander, Wilson, JCP 54, 4127 (1971).
- (32) Mulliken, JCP 55, 288 (1971).
- (33) Potts, Price, TFS 67, 1242 (1971).
- (34) Sorem, Levenson, Schawlow, PL A 37, 33 (1971).
- (35) Tellinghuisen, quoted in (32).
- (36) Wieland, quoted in (32).
- (37) Brewer, Tellinghuisen, JCP 56, 3929 (1972).
- (38) Broyer, Lehmann, PL A 40, 43 (1972).
- (39) Le Roy, CJP 50, 953 (1972).
- (40) Levenson, Schawlow, PR A 6, 10 (1972).
- (41) Shotton, Chapman, JCP 56, 1012 (1972).
- (42) Capelle, Broida, JCP 57, 5027 (1972).
- (43) Chapman, Bunker, JCP 57, 2951 (1972).
- (44) Solarz, Levy, CPL 17, 35 (1972).
- (45) Sorem, Hänsch, Schawlow, CPL 17, 300 (1972).
- (46) Tellinghuisen, JCP 57, 2397 (1972).
- (47) Wieland, Tellinghuisen, Nobs, JMS 41, 69 (1972).
- (48) Kiefer, Bernstein, JMS 43, 366 (1972).
- (49) Barrow, Broyd, Pederson, Yee, CPL 18, 357 (1973).
- (50) Barrow, Yee, JCS FT II 69, 684 (1973).
- (51) Brown, Burns, Le Roy, CJP 51, 1664 (1973).
- (52) Capelle, Broida, JCP 58, 4212 (1972).
- (53) Child, JMS 45, 293 (1973).
- (54) Clear, Wilson, JMS 47, 39 (1973).
- (55) Comes, Nielsen, Schwarz, JCP 58, 2230 (1973).
- (56) Higginson, Lloyd, Roberts, CPL 19, 480 (1973).
- (57) Keller, Broyer, Lehmann, CR B 277, 369 (1973).
- (58) Le Roy, in "Molecular Spectroscopy", Vol. 1, p. 113. The Chemical Society (1973).

(Continued on p. 337)

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
								Design.	v ₀₀		
¹²⁷ I ⁷⁹ Br											
62000 - 77000		μ = 48.658793 ₇ D ₀ ⁰ = 1.817 ₆ eV ^a I.P. = 9.85 eV ^b								JAN 1977 A	
		{ Fragments of several Rydberg series converging to X ² Π _{3/2} and ² Π _{1/2} of IBr ⁺ . Tentative assignments. The three strongest series join on to E, H, J, resp..								(18)	
J	65793	[267]	H					J ← X,	65792	H	(18)
H	(64092)	(290)	H					H ← X,	(V) (64103) ^c	H	(14)*
G	(60877)	(280)	H					G ← X,	(V) (60883) ^c	H	(14)*
F	56349	[310]	H					F ↔ X, ^d	V 56370	H	(3)(5)(14)*
E	51677	[314]	H					E ↔ X, ^e	V 51700	H	(3)(5)(14)*
D	(38849)	90.2	H	0.15				D → A, ^f	R (26476)	H	(5)(6)
		Diffuse emission bands from 19000 to 29000 and 36000 to 43000 cm ⁻¹ .									(4)
		Fragments of three emission band systems near 18600, 22300, and 24500 cm ⁻¹ .									(6)
		Weak continuous absorption with maximum at 37000 cm ⁻¹ .						(B' ← X)		}	(12)(14)
		Strong continuous absorption with maximum at 20200 cm ⁻¹ . ^g						(B ← X)			
B' 0 ⁺	(60)	{ Potential well resulting from an avoided intersection of a repulsive 0 ⁺ state with B ³ Π ₀₊ ; see (2)(10)(19)(23). ^h						B' ← X,		R	(2)(10)*

IBr: ^aFrom the convergence of A $^3\Pi_1$; see ^l.

^bVertical potential from the photoelectron spectrum (17); vibrational structure not resolved. From the temperature dependence of the photo-ion yield curve in the threshold region (17a) conclude that the adiabatic potential is probably 9.79 eV.

^c(18) give 63573 and 60624 as 0-0 bands of these systems [called F-X, and E-X, resp., by (14)]; the band intervals seem to fit better with the choice made here.

^dFormerly called D-X.

^eFormerly called C-X. An extended resonance series excited by the 1849 Å Hg line (1) may originate from a high level ($v'=8?$) of E.

^fThe analysis of this system was based on the old (2) numbering of the A-X system. The shift in the numbering by one unit established by (9) means either that the $v''=0$ column has to be omitted from the D-A Deslandres table of (6), and thus $v_{00} = 26340$, or that the ΔG° values of (6) are systematically higher than those of (2) and (9). Our choice of v_{00} [from (6)] corresponds to the latter alternative.

IBr (continued):

^gAbsorption in the continuum at $\nu \approx 33000 \text{ cm}^{-1}$ produces predominantly excited $\text{Br } ^2\text{P}_{\frac{1}{2}}$ atoms [diabatic dissociation, see (14)]. By contrast, absorption at 18830 cm^{-1} , i.e. closer to the region of the avoided crossing of the two 0^+ curves, leads mainly to ground state $\text{Br } ^2\text{P}_{\frac{1}{2}}$ atoms [adiabatic dissociation (15)]. See also the discussion in (19a).

^hVibrational levels of this state, some sharp, others diffuse, have been observed (2) from 17215 cm^{-1} (relative to $X ^1\Sigma, v=0$) to 18315 cm^{-1} , i.e. to within 30 cm^{-1} of the

limit $I(^2\text{P}_{\frac{3}{2}}) + \text{Br}(^2\text{P}_{\frac{1}{2}})$. The vibrational numbering is still undecided; (10), following (2), assigns $v=8$ to the lowest observed level, (19) suggest $v=2$, while (22) prefer $v=5$. Narrow J regions of a number of levels have been analyzed by (10); B_v varies from $0.03226 \text{ (I}^{81}\text{Br)}$ for $v=8$ in the numbering of (10) to $0.0229 \text{ (I}^{79}\text{Br)}$ for $v=27$. The levels $v=25$ of I^{81}Br and $v=26$ of I^{79}Br have also been observed in the magnetic rotation spectrum (7).

(references on p. 339)

I_2 (continued):

- (59) Singh, Tellinghuisen, JMS 47, 409 (1973).
- (60) Tellinghuisen, JCP 58, 2821 (1973).
- (61) Tellinghuisen, JCP 52, 849 (1973).
- (62) Yee, CPL 21, 334 (1973).
- (63) Youmans, Hackel, Ezekiel, JAP 44, 2319 (1973).
- (64) Broyer, Vigué, Lehmann, CPL 22, 313 (1973).
- (65) Ruben, Kukolich, Hackel, Youmans, Ezekiel, CPL 22, 326 (1973).
- (66) Le Roy, CJP 52, 246 (1974).
- (67) Verma, Le Roy, JCP 61, 438 (1974).
- (68) Vigué, Broyer, Lehmann, JP B 7, L158 (1974).
- (69) Wallenstein, Paisner, Schawlow, PRL 32, 1333 (1974).
- (70) Wei, Tellinghuisen, JMS 50, 317 (1974).
- (71) Williams, Rousseau, Dworetzky, PRL 32, 196 (1974).
- (72) Tellinghuisen, CPL 22, 359 (1974).
- (73) Brown, Burns, CJP 52, 1862 (1974).
- (74) Bunker, Hanes, CPL 28, 377 (1974).
- (75) Howard, Andrews, JRS 2, 447 (1974).

- (76) Paisner, Wallenstein, JCP 61, 4317 (1974).
- (77) Rousseau, Williams, PRL 33, 1368 (1974).
- (78) Brith, Rowe, Schnepp, Stephens, CP 2, 57 (1975).
- (79) Broyer, Lehmann, Vigué, JP(Paris) 36, 235 (1975).
- (80) Broyer, Vigué, Lehmann, JCP 63, 5428 (1975).
- (81) Hackel, Casleton, Kukolich, Ezekiel, PRL 35, 568 (1975).
- (82) Rousseau, JMS 58, 481 (1975).
- (83) Tellinghuisen, PRL 34, 1137 (1975).
- (84) Tesic, Pao, JMS 57, 75 (1975).
- (85) Vigué, Broyer, Lehmann, JCP 62, 4941 (1975).
- (86) Broyer, Vigué, Lehmann, JCP 64, 4793 (1976).
- (87) Gouedard, Broyer, Vigué, Lehmann, PRL 36, 906, 996 (1976).
- (88) Gouedard, Broyer, Vigué, Lehmann, CPL 43, 118 (1976).
- (89) Hays, Hoffman, Tisone, CPL 32, 353 (1976).
- (90) Tellinghuisen, JMS 62, 294 (1976).
- (91) Gerstenkorn, Luc, Perrin, JMS 64, 56 (1977).
- (92) Ashby, private communication (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{127}\text{I}^{79}\text{Br}$ (continued)										
B $3\Pi_0^+$	16168	142.5	Z	2.57 ⁱ	0.0432 ^{jk}	0.0005 ₃	$D_2 = 2.2$	2.83	B \leftarrow X, R 16104 ^j	Z (2)(11)
A $3\Pi_1$	12350	138		1.7 ^l	$B_9 = 0.03803^m$		$D_9 = 3.0^m$		A \leftrightarrow X, ⁿ R 12285 ^o	(2)(9)* (13)*
X $1\Sigma^+$	0	268.64 ₀ ^p	Z	0.814 ₀ ^q	0.0568325 ₂ ^r	0.0001969 ₀ ^s	(1.02)	2.46898 ₉	Raman sp. ^t Microwave sp. ^u	(16) (20)
$^{127}\text{I}(^{79})\text{Br}^+$										
B $2\Sigma^+$	(31050)	$D_0^0 = 2.42 \text{ eV}^a$							JAN 1977	
A $2\Pi_{1/2}$	(20410)									
A $2\Pi_{3/2}$	(17260)									
X $2\Pi_{1/2}$	4600									
X $2\Pi_{3/2}$	0									
$^{127}\text{I}(^{79})\text{Br}^-$										
						$D_0^0 = 1.1_2 \text{ eV}^b$	I.P. = 2.6 ₇ eV ^c		JAN 1977	

IBr (continued):

ⁱ $\omega_e y_e = -0.11$; from $v=2,3,4$, including data for I^{81}Br .^jExtrapolated from data with $v'=2,3,4$.^kBands with $v'=5$ are diffuse, presumably because of pre-dissociation into the intersecting 0^+ state from $2P_{3/2} + 2P_{3/2}$. Higher levels are not observed; see, however, B 0^+ .^l $\omega_e y_e = -0.02$; the constants represent the levels $v' = 5 \dots 16$ (9)(13), vibrational numbering confirmed by theobserved isotope shifts (9). Levels have been identified up to $v=43$, convergence at 14660 cm^{-1} .^m B_v and D_v values from $v=9$ to 30 are listed by (9). The Λ -type doubling constant $q [\approx B(R,P) - B(Q)]$ for $v=14$ is $+10 \times 10^{-6}$ and increases to 42×10^{-6} for $v=29$.ⁿAn extended magnetic rotation spectrum has been observed by (7).^oExtrapolated from data with $v' \geq 5$.

IBr (continued):

^pThese vibrational constants from laser-excited fluorescence data (24) differ only very slightly from the earlier constants of (9).

^q $\omega_e y_e = -0.0017$.

^rMicrowave value of (20), in good agreement with the less accurate values from the electronic spectrum (9)(24). An earlier microwave value by (8) was clearly erroneous.

^s $\gamma_e = -4.7 \times 10^{-7}$.

^tResonance Raman spectra in argon matrices (21).

^uIodine and bromine eqQ values for $v=0,1,2$.

- (1) Loomis, Allen, PR 33, 639 (1929).
- (2) Brown, PR 42, 355 (1932).
- (3) Cordes, Sponer, ZP 79, 170 (1932).
- (4) Asundi, Venkateswarlu, IJP 21, 77 (1947).
- (5) Haranath, Rao, IJP 31, 368 (1957).
- (6) Venkateswarlu, Verma, PIAS A 47, 150, 161 (1958).
- (7) Eberhardt, Cheng, Renner, JMS 3, 664 (1959).
- (8) Jaseja, JMS 5, 445 (1960).
- (9) Selin, AF 21, 479 (1962).
- (10) Selin, AF 21, 529 (1962).
- (11) Selin, Söderborg, AF 21, 515 (1962).
- (12) Seery, Britton, JPC 68, 2263 (1964).
- (13) Clyne, Coxon, JMS 23, 258 (1967).
- (14) Donovan, Husain, TFS 64, 2325 (1968).
- (15) Busch, Mahoney, Morse, Wilson, JCP 51, 837 (1969).
- (16) Holzer, Murphy, Bernstein, JCP 52, 399 (1970).
- (17) Potts, Price, TFS 67, 1242 (1971).
- (17a) Dibeler, Walker, McCulloh, Rosenstock, IJMSIP 7, 209 (1971).
- (18) Donovan, Robertson, SpL 5, 361 (1972).

IBr (continued):

- (19) Child, Bernstein, JCP 59, 5916 (1973).
- (19a) Coxon, in "Molecular Spectroscopy", Vol. 1, p. 177. The Chemical Society (1973).
- (20) Tiemann, Möller, ZN 30 a, 986 (1975).
- (21) Wight, Ault, Andrews, JMS 56, 239 (1975).
- (22) Couillaud, Ducasse, Garrido, Joly, JP B 9, 2091 (1976).
- (23) Faist, Bernstein, JCP 64, 2971 (1976).
- (24) Weinstock, JMS 61, 395 (1976).

IBr⁺, IBr⁻:

^aFrom $D_0^0(\text{IBr}) + \text{I.P.}(\text{I}) - \text{I.P.}(\text{IBr})$.

^bFrom $D_0^0(\text{IBr})$ and the electron affinities of Br and IBr.

^cFrom endoergic charge transfer, average of three values (2)(3).

- (1) See ref. (17) of IBr.
- (2) Chupka, Berkowitz, Gutman, JCP 55, 2724 (1971).
- (3) Baede, Physica 59, 541 (1972).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁸ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
								Design.	v ₀₀		
¹²⁷ I ³⁵ Cl		μ = 27.4146708 D ₀ ⁰ = 2.1531 eV ^a I.P. = 10.08 eV ^b								JAN 1977 A	
		Fragments of many Rydberg series in the absorption spectrum above 60000 cm ⁻¹ have been observed and tabulated by (23); see also (19). The intensities in these series are most irregular, possibly because of perturbations by valence states in this region. The Rydberg series are believed to converge to two limits at 81362 and 85996 cm ⁻¹ corresponding to the ² Π _{3/2} and ² Π _{1/2} , v=0 components of the ground state of ICl ⁺ .								(23)*	
L	71006	[420]	H	Strong progression, F←X of (14), n ₅ of (23).				L←X, V 71024		(14)* (23)*	
G	66484	[421]	H	Strong progression, E←X of (14), g ₅ of (23).				G←X, V 66503	H	(14)* (23)*	
		Extensive system of absorption bands in the region 60250-63300 cm ⁻¹ , not yet analyzed.								(23)	
F	58167	[445]	H	Extensive band system, formerly D-X, b ₆ of (23).				F↔X, V 58198	H	(2)(7)(14)* (23)*	
E	53477	[434]	H	Extensive band system, formerly C-X, a ₆ of (23).				E↔X, V 53502	H	(2)(7)(14)* (23)*	
		Continuous absorption with maximum at 41600 cm ⁻¹ .								(11)	
D	37585	173.2	H	1.1	Extensive band system.			D→A, ^c R 23824	H	(7)*	
		Diffuse emission bands between 18700 and 27100 cm ⁻¹ .								(4)	
		Continuous absorption with maximum at 21000 cm ⁻¹ . ^d								(11)	
B' 0 ⁺	(18157)	[32]	{ Potential well arising from the avoided crossing of the "original" B ³ Π ₀ ⁺ curve going to I(² P _{3/2}) + Cl(² P _{3/2}) and the repulsive 0 ⁺ curve coming from unexcited atoms; see also (20b). ^e						B'←X, R 17981	H	(1)
B ³ Π ₀ ⁺	17363.1	221.1 ^f	Z	9.62	0.0872 ^{fg}	0.0017	(10)	2.66	B←X, ^h R 17279.5 ^f	Z	(1)(10)
A ³ Π ₁	13742	212.3 ⁱ	H	2.39 ^j	0.084832 ^k		(5.4)	2.6923	A ^l ↔X, ^m R 13656 ⁱ	H	(3)* (8)(10) (12)*
X ¹ Σ ⁺	0	384.29 ₃	Z	1.501	0.1141587 ⁿ	0.0005354	(4.03)	2.32087 ₈	Infrared sp. ^o Raman sp. ^p Microwave sp. ^o		(6) (15) (5)(20)

IC₂: ^aFrom the convergence limit of A $^3\Pi_1$, see ^j.
^bAverage value obtained by photoelectron spectroscopy (17)(18) and photoion mass-spectrometry (18a).
^cConstants of (7) for the lower state ($\omega_e = 209.7$, $\omega_e x_e = 1.9$) are not in agreement with the work of (12) and (21) concerning the A $^3\Pi_1$ state; see (12). This system was also observed in fluorescence following two-step laser excitation D \leftarrow A \leftarrow X (22). (Note that ν_e given by (7) does not match their observed ν_{00} .)
^dAt least partly due to B \leftarrow X; see the discussion in (20a).
^eThere are fragments of fairly sharp branches at places corresponding to extrapolated levels of B $^3\Pi_0$ +.
^fExtrapolated from data with $\nu' = 1, 2, 3$.
^g $\nu' = 4$ is strongly predissociated and gives rise to broad, diffuse absorption bands; no higher levels are observed. At high resolution (25) even $\nu' = 3$ shows appreciable broadening of the individual lines which rapidly increases above $J' = 37$ and is presumably caused by predissociation into the O $^+$ state arising from $^2P_{3/2} + ^2P_{3/2}$; see B' O $^+$. The non-radiative lifetime varies from ~ 0.2 ns at low J to 0.02 ns at J=42 (25).
^hThe f value is estimated to be 0.0026 corresponding to a radiative lifetime of 1 μ s (25).
ⁱVibrational constants from (12) whose measurements of the I + Cl chemiluminescence spectrum include bands with $\nu' = 1 \dots 18$. (21), extrapolating from the data (zero lines) of (10) for $3 \leq \nu' \leq 19$, obtain $\nu_{00} = 13655.23$. Earlier, from band origins with $7 \leq \nu' \leq 19$, (10) derived $\omega_e = 209.111$, $\omega_e x_e = 1.886$, $\omega_e y_e = -0.03558$, $\nu_{00} = 13660.29$. See ^j.
^j $\omega_e y_e = -0.012$ (12). T_v values for 38 levels ($\nu \geq 3$) are listed in (10). There is a strong vibrational perturbation above $\nu = 34$, but the last few levels are again regular and converge to 17366.0 cm^{-1} .

^kB $_e$, as well as B $_0 = 0.084583$, B $_1 = 0.083995$, B $_2 = 0.083308$, have been extrapolated by (21) from the B $_v$ values of (10) for $3 \leq v \leq 19$. B $_v$ values up to $v = 40$ are tabulated in (10). The Λ -type doubling constant q [$\approx B(R,P) - B(Q)$] increases from $+1.32 \times 10^{-5}$ for $v = 10$ to $+11.0 \times 10^{-5}$ for $v = 27$, but the doubling becomes irregular at higher v values (10). The dipole moment in A $^3\Pi_1$ varies from 2.00 D at $v = 7$ to 0.6 D at $v = 27$ (21); sign opposite to that in X $^1\Sigma^+$. RKR potential curve (20a).
^lFluorescence lifetimes of 110 and 76 μ s have been measured (16) following laser excitation at 6068 and 5922 Å, resp..
^mMagnetic rotation spectrum (9); its intensity drops sharply above $\nu' = 28$. See also (13). Laser induced fluorescence series in argon matrix (24).
ⁿFrom the microwave spectrum (20); in excellent agreement with the much earlier values from the electronic spectrum (3).
^o $\mu_{el}(\nu = 0) = 1.24 \text{ D}$ (20); dipole derivative 2.1 D/Å (6). Electric quadrupole coupling constants for I and Cl in (20), also iodine spin-rotation constant.
^pResonance Raman spectrum in argon matrix (24).

- (1) Brown, Gibson, PR 40, 529 (1932).
 - (2) Cordes, Spomer, ZP 79, 170 (1932).
 - (3) Curtis, Patkowski, PTRSL A 232, 395 (1934).
 - (4) Asundi, Venkateswarlu, IJP 21, 76 (1947).
 - (5) Townes, Merritt, Wright, PR 73, 1334 (1948).
 - (6) Brooks, Crawford, JCP 23, 363 (1955).
 - (7) Haranath, Rao, IJP 31, 156 (1957).
 - (8) Hulthén, Johansson, Pilsäter, AF 14, 31 (1958).
 - (9) Eberhardt, Cheng, Renner, JMS 3, 664 (1959).
 - (10) Hulthén, Järlsäter, Koffman, AF 18, 479 (1960).
- (continued on p. 343)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{127}\text{I}(35)\text{Cl}^+$		$D_0^0 = 2.52 \text{ eV}^a$							JAN 1977	
B ($^2\Sigma$)	(33550)	[390]	} From the photoelectron spectrum (band maxima) (1).							
A ($^2\Pi$)	(22420)									
X $\begin{matrix} 2\Pi_{1/2} \\ 2\Pi_{3/2} \end{matrix}$	$\begin{matrix} 4680 \\ 0 \end{matrix}$									
$^{127}\text{I}^{19}\text{F}$		$\mu = 16.5245715$	$D_0^0 = 2.87_9 \text{ eV}^a$		$\text{I.P.} = (10.5) \text{ eV}^b$			JAN 1977 A		
B $^3\Pi_0^+$	19052.2 ₄	411.34 ^c Z	2.825 ^d	0.2272 ₁ ^e	0.00139 ₈ ^f	0.2 ₈	2.118 ₉	B \rightarrow X, ^g R 18952.8 ₆ Z	(2)* (3)* (7)*	
A $^3\Pi_1$	15706	380.5 H	3.8					A \rightarrow X, R 15591 H	(7)*	
X $^1\Sigma^+$	0	610.24 ^c Z	3.123 ^h	0.279710 ₈	0.001873 ₄ ⁱ	0.237	1.90975 ₉	Microwave sp. ^j	(5)(6)	
$(^{115})\text{In}_2$		$(\mu = 57.451938) \quad D_0^0 = 1.0_1 \text{ eV}^a$							APR 1977	
		R and V shaded bands in emission from 16800 to 20000 cm^{-1} ($w' \approx 115$, $w'' \approx 142$) and in absorption ^b from 26000 to 28000 cm^{-1} .							(3)	

ICl (continued):

- (11) Seery, Britton, JPC 68, 2263 (1964).
- (12) Clyne, Coxon, PRS A 298, 424 (1967).
- (13) Stalder, Eberhardt, JCP 47, 1445 (1967).
- (14) Donovan, Husain, TFS 64, 2325 (1968).
- (15) Holzer, Murphy, Bernstein, JCP 52, 399 (1970).
- (16) Holleman, Steinfeld, CPL 12, 431 (1971).
- (17) Potts, Price, TFS 67, 1242 (1971).
- (18) Cornford, Thesis (Univ. of British Columbia, 1971).
- (18a) Dibeler, Walker, McCulloh, Rosenstock, IJMSIP 7, 209 (1971).
- (19) Donovan, Robertson, SpL 5, 281 (1972).
- (20) Herbst, Steinmetz, JCP 56, 5342 (1972).
- (20a) Coxon, in "Molecular Spectroscopy", Vol. 1, p. 177. The Chemical Society (1973).
- (20b) Child, Bernstein, JCP 59, 5916 (1973).
- (21) Cummings, Klemperer, JCP 60, 2035 (1974).
- (22) Barnes, Moeller, Kircher, Verber, APL 24, 610 (1974).
- (23) Venkateswarlu, CJP 53, 812 (1975).
- (24) Wight, Ault, Andrews, JMS 56, 239 (1975).
- (25) Olson, Innes, JCP 64, 2405 (1976).

ICl⁺: ^aFrom $D_0^0(\text{ICl}) + \text{I.P.}(\text{I}) - \text{I.P.}(\text{ICl})$.

(1) See ref. (17) of ICl.

IF: ^aThis is the value of (7) and (8) based on a discussion of the vibrational levels in A $^3\Pi_1$ and B $^3\Pi_0^+$; an upper limit of 2.894 eV follows from the observed predissociation in B. (4) suggest $D_0^0 = 2.54$ eV on the basis of comparisons with other interhalogens.

^bElectron impact appearance potential (1).

^cThe vibrational constants for both B $^3\Pi_0^+$ and X $^1\Sigma^+$ have

IF (continued):

been recalculated from the data of (2). Similar revised constants for the ground state may be found in (8). Additional higher order constants are needed to represent the B state levels above $v=6$.

^d $w_e y_e = -0.0744$; see ^c.

^eOnset of predissociation at $J=45$ of $v=11$ (23341 cm^{-1}).

^f $r_e = -0.000082$.

^gRKR Franck-Condon factors, variation of transition moment with r (7).

^h $w_e y_e = -0.00347$.

ⁱ $r_e = -0.0000027$.

^jIodine hyperfine coupling constants (6).

- (1) Irsa, Friedman, JINC 6, 77 (1958).
- (2) Durie, CJP 44, 337 (1966).
- (3) Clyne, Coxon, Townsend, JCS FT II 68, 2134 (1972).
- (4) See ref. (20b) of ICl.
- (5) McGurk, Flygare, JCP 59, 5742 (1973).
- (6) Tiemann, Hoeft, Törring, ZN 28 a, 1405 (1973).
- (7) Birks, Gabelnick, Johnston, JMS 57, 23 (1975).
- (8) Coxon, CPL 33, 136 (1975).

In₂: ^aThermochemical value (mass-spectrom.) (2) (4).

^bSee also the earlier work of (1).

- (1) Wajnkranz, ZP 104, 122 (1936/7).
- (2) De Maria, Drowart, Inghram, JCP 31, 1076 (1959).
- (3) Ginter, Ginter, Innes, JPC 69, 2480 (1965).
- (4) Gingerich, Blue, 18th Annual Conference on Mass Spectrometry and Allied Topics. San Francisco (June 1970).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{115}\text{In}^{81}\text{Br}$		$\mu = 47.480276$ $D_0^0 = 3.9_g \text{ eV}^a$ I.P. = 9.09 eV^b								JAN 1977 A
C $^1\Pi$ (34000)		Fluctuation bands with various v'' ; shallow upper potential curve.						C \leftarrow X, 35053 ^c		(1)*
B $^3\Pi_1$ 27382.2	218.0 ^d H 1.60							B \leftrightarrow X, v_R 27380.5 H	(1)* (5)*	
A $^3\Pi_0^+$ 26596.0	227.4 ^d H 1.58							A \leftrightarrow X, v 26599.0 H	(1)* (5)*	
X $^1\Sigma^+$ 0	221.0 H 0.65	0.0548944 ^e	0.0001862 ^e	(1.35)	2.54318	Microwave sp. ^f		(2)		
$^{115}\text{In}^{(79)}\text{Br}^+$		$D_0^0 = 0.6_g \text{ eV}^g$								JAN 1977
B ($^2\Sigma$) (26500)	} From the photoelectron spectrum (adiabatic potentials)(6). ^h									
A ($^2\Pi$) (4300)										
X ($^2\Sigma$) 0										
$^{115}\text{In}^{35}\text{Cl}$		$\mu = 26.8097927$ $D_0^0 = 4.44 \text{ eV}^a$ I.P. = 9.51 eV^b								JAN 1977
		Continuous absorption, $\sim 47600 \text{ cm}^{-1}$.								(1)(3)
		Narrow continuum, maximum at 38260 cm^{-1} .								(1)(2)* (3)
D		177.3	H ^Q 12.6					D \leftarrow X,		(1)(2)* (3)*
C $^1\Pi$ 37483.6		339.4 ^d H 2.1	[0.1152]		[2.4]	[2.336]		C \leftrightarrow X, R 37410.7 H ^Q		(1)(2)* (3)*
B $^3\Pi_1$ 28560.2								B \leftrightarrow X, v 28570.9 H		(2)* (7) (14)*
A $^3\Pi_0^+$ 27764.7		340.3 H 2.0	0.1155	0.000654	6.5	2.333		A \leftrightarrow X v 27775.9 H		(2)* (7)* (14)*
X $^1\Sigma^+$ 0		317.4 H ^Q 1.01	0.1090580	0.0005178 ^e	(5.14)	2.401169		Microwave sp. ^f		(5)(9)(10)
$^{115}\text{In}^{(35)}\text{Cl}^+$		$D_0^0 = 0.72 \text{ eV}^g$								JAN 1977
B ($^2\Sigma$) (26700)	} From the photoelectron spectrum (adiabatic potentials)(12). ^h									
A ($^2\Pi$) (5300)										
X ($^2\Sigma$) 0										

InBr, InBr⁺:

^aFrom thermochemical data and spectroscopic evidence about the ¹Π and ³Π excited states; see (3). In good agreement with 4.0₂ eV obtained by flame photometry (4).

^bAdiabatic potential from the photoelectron spectrum (6); vertical potential 9.41 eV.

^cVertical transition from v''=0.

^dConstants for ¹¹⁵In⁷⁹Br are given by (5) who propose small changes in the vibrational numbering of the B-X bands observed by (1).

^eCalculated from the rotational constants for the ¹¹⁵In⁷⁹Br isotope (2).

^fElectric quadrupole coupling constants.

^gFrom D₀⁰(InBr) + I.P.(In) - I.P.(InBr).

^hThe ²Π photoelectron peak is very broad with a maximum at 10.20 eV (²Π_{1/2}?) and a shoulder at ~9.8 eV (²Π_{3/2}?). These vertical potentials are close to the dissociation limits In⁺(¹S) + Br(²P_{1/2}, ²P_{3/2}) at 10.2₄ and 9.7₈ eV, respectively, and seem compatible with the predicted instability or near instability of A ²Π.

(1) Wehrli, Miescher, HPA 6, 457 (1933); 7, 298 (1934).

(2) Barrett, Mandel, PR 109, 1572 (1958).

(3) Barrow, TFS 56, 952 (1960).

(4) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(5) Lakshminarayana, Haranath, IJP 44, 504 (1970).

(6) Berkowitz, Dehmer, JCP 57, 3194 (1972).

InCl, InCl⁺:

^aFrom thermochemical data and spectroscopic evidence about the ¹Π excited state (6); 4.5₁ eV by flame photometry (8).

InCl, InCl⁺ (continued):

^bAdiabatic potential from the photoelectron spectrum (12); vertical potential 9.75 eV.

^cThe rotational analysis of v=0 by (3) is probably not correct [see (4), p.967-8]. Predissociation for v ≥ 1; the diffuseness is stronger for v=2 than for v=1.

^dConstants from (2), slightly different constants in (14).

^eγ_e = + 8.4 × 10⁻⁷.

^fμ_{el}(v=0) = 3.79 D (13). Quadrupole coupling constants (11).

^gFrom D₀⁰(InCl) + I.P.(In) - I.P.(InCl).

^hThe maximum (vertical potential) of the very broad ²Π peak is at 10.85 eV, i.e. the ²Π potential curve in the Franck-Condon region has risen ~0.6 eV above its dissociation limit In⁺(¹S) + Cl(²P).

(1) Miescher, Wehrli, HPA 6, 256 (1933).

(2) See ref. (1) of InBr, InBr⁺.

(3) Frosli, Winans, PR 72, 481 (1947).

(4) Barrow, Glaser, Zeeman, PPS A 68, 962 (1955).

(5) See ref. (2) of InBr, InBr⁺.

(6) See ref. (3) of InBr, InBr⁺.

(7) Youngner, Winans, JMS 4, 23 (1960).

(8) See ref. (4) of InBr, InBr⁺.

(9) Hoeft, ZP 163, 262 (1961).

(10) Delvigne, de Wijn, JCP 45, 3318 (1966).

(11) Schenk, Tiemann, Hoeft, ZN 25 a, 1827 (1970).

(12) See ref. (6) of InBr, InBr⁺.

(13) Tiemann, Hoeft, Törring, ZN 27 a, 869 (1972).

(14) Ashrafunnisa, Rao, Murthy, Rao, Physica 73, 421 (1974).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{115}\text{In}^{19}\text{F}$											
$\mu = 16.3028614$ $D_0^0 = 5.2_5 \text{ eV}^a$											
Unidentified weak system in emission consisting of two sequences of R shaded bands; $\Delta G'(\frac{1}{2}) = 550$, $\Delta G''(\frac{1}{2}) = 610$. R and Q heads.											
Weak system.											
D	[47803]	463.9	H^Q 7.35 ^b	0.2674	0.0047 ₂	0.036	1.966	D \leftarrow X, R 47536	H	(2)	
C	1_{Π} 42809.2	572.2 ₅	H^Q 2.63 ^c	0.2736 ₂ ^d	0.0020 ₄	(0.025)	1.944 ₀	C \leftrightarrow X, R _V 42772.3	Z	(1)(3)(10)*	
B	3_{Π_1} 31255.7 ₄	575.2	(Z) 3.67 ₆	0.2732 ₀ ^d	0.0020 ₂	(0.025)	1.945 ₅	B \leftrightarrow X, V 31274.1 ₈	Z	(1)(2)(3)	
A	3_{Π_0+} 30445.8 ₆	535.3 ₅	Z 2.6 ₄	0.262324 ₁	0.0018797 ₇ ^e	0.0252	1.985396	A \leftrightarrow X, V 30465.5 ₂	Z	(1)(2)(3)	
X	1_{Σ^+} 0							Microwave sp. ^f		(7)(8)	
								Mol. beam el. reson. ^g		(9)	
$^{115}\text{In}^1\text{H}$											
$\mu = 0.99906241$ $D_0^0 = 2.48 \text{ eV}^a$											
Open band structure in absorption from 40000 to 42900 cm^{-1} , no prominent heads.											
A	1_{Π} (22655)	[141.7]	Z ^b	[3.850] ^c	^d	[389]	[2.093]	A \leftarrow X, R 22016.9	Z	(4)(5)	
a	3_{Π} { 2 (17800)	[1300.9] ^e	Z	5.489 ^{ef}	0.332	[34.6]	1.753	a { \rightarrow X, V _R 17780.9	Z	(6)	
	1 16941.6 ₁	1415.1 ₁ ^e	Z 43.5 ₅ ^g	5.399 ₆ ^{ehijk}	0.235 ₆ ^h	[32.1] ^h	1.7678		\leftrightarrow X, R _V 16904.9 ₈	Z	(1)(4)(6)
	0 ⁺ 16278.1 ₅	1458.5 ₇ ^e	Z 61.0 ₃ ^l	5.329 ^{eik}	0.246 ₈ ^m	[27.7] ⁿ	1.779 ₄		\leftrightarrow X, R _V 16259.6 ₈	Z	(1)(6)
	0 ⁻ (16230)	[1303.4 ₂] ^e	Z	5.349 ^e	0.326	[28.1] ^o	1.776		\rightarrow X, V _R 16211.5 ₃	Z	(10)
a'	3_{Σ^+}	{ Not observed, but suggested (12) as the state responsible for anomalies in the A-type doubling of 3_{Π_1} and for the predissociation of all 3_{Π} components.									
X	1_{Σ^+} 0	1476.0 ₄	Z 25.61 ^p	4.994 ₅ ^k	0.142 ₈ ^q	22.3 ^r	1.8380				
$^{115}\text{In}^2\text{H}$											
$\mu = 1.97940604$ $D_0^0 = 2.51 \text{ eV}^s$											
A	1_{Π} (22600)	[178.2]	Z ^t	[2.096] ^u	^v	[42.6]	[2.016]	A \leftarrow X, R 22167.1	Z	(5)	
a	3_{Π} { 1 16933	[950.03]	Z ^w	2.724 ^j	0.078 ^x	[8.2]	1.768 ₂	a { \leftarrow X, V _R 16922.40	Z	(5)	
	0 ⁺ (16270)	[967.79]	Z	2.722	0.112	[7.9]	1.769		\leftarrow X, V 16273.99	Z	(5)
X	1_{Σ^+} 0	1048.2 ₄	Z 12.3 ₇	2.523	0.051	[5.8]	1.837 ₃				

InF: ^aThermochemical value (mass-spectrom.)(6). Flame photometry gives 5.4 eV (5).

^b $w_e y_e = -0.5$. This state may have a potential maximum of ~ 0.21 eV (4)(6).

^c $w_e y_e = -0.095$.

^dFrom the B' - B" values of (3) combined with B" from the microwave spectrum.

^e $\gamma_e = +0.0000049_7$.

^f $\mu_{el}(v=0) = 3.40$ D (8).

^gHyperfine interaction constants.

(1) Welti, Barrow, Nature 168, 161 (1951); PPS A 65, 629 (1952).

(2) Barrow, Jacquest, Thompson, PPS A 67, 528 (1954).

(3) Barrow, Glaser, Zeeman, PPS A 68, 962 (1955).

(4) Barrow, TFS 56, 952 (1960).

(5) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(6) Murad, Hildenbrand, Main, JCP 45, 263 (1966).

(7) Lovas, Törring, ZN 24 a, 634 (1969).

(8) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 1029 (1970).

(9) Hammerle, Van Ausdal, Zorn, JCP 57, 4068 (1972).

(10) Nampoori, Kamalasanan, Patel, JP B 8, 2841 (1975).

In¹H, In²H:

^aFrom the predissociations in A ¹ Π and a ³ Π .

^b $\Delta G(3/2) = 80.8$.

^cA-type doubling, $\Delta v_{ef}(v=0) = +0.0047$ J(J+1). Breaking off due to predissociation above J' = 9, 7, 4 in v' = 0, 1, 2, respectively; the limiting curve intersects the ordinate axis near 22250 cm⁻¹ above X ¹ $\Sigma(v=0, J=0)$. A few additional diffuse lines have been observed as well as fragments of an "extra" band; see ^d.

^dB₁ = 1.915, B₂ = 1.363. D_v values are also given (4), but

In¹H, In²H (continued):

these constants are not sufficient to reproduce the levels of this perturbed state. Zeeman effect studies (7).

^eEffective constants determined by (6)(10). For a more rigorous treatment of the fine structure of a ³ Π see (12).

^fPredissociation in v=0 above J=26 (³ Π^-) and 27 (³ Π^+), in v=1 above J=17 (³ Π^+). The break-off points are in agreement with the limiting curve of dissociation for ³ Π_1^+ (6).

^g $w_e y_e = -13.14$.

^hAverage constants for ³ Π_1^+ and ³ Π_1^- ; $\gamma_e = -0.056_7$. The Λ -type doubling is irregular, see (12), and may be caused by the unobserved a' ³ Σ^+ state. Zeeman effect studies (7).

ⁱThe ³ Π_1 and ³ Π_0 components have nearly identical limiting curves of predissociation; the derived dissociation limit at 20125 cm⁻¹ above X ¹ Σ , v=0, J=0, appears to correspond to a potential maximum at ~ 3.3 Å (6). Possible correlations of the low-lying states of InH with those of the separated atoms have been discussed by (8) and, more recently, by (12).

^jThe hyperfine structure of J=1 has been investigated both experimentally (4)(5)(11) and theoretically (9)(13).

^kRKR potential curves (8).

^l $w_e y_e = -6.83$.

^m $\gamma_e = -0.039_0$.

ⁿ $H_0 = -3.76 \times 10^{-8}$. $|D_v|$ and $|H_v|$ increase rapidly with v.

^o $H_0 = -2.9 \times 10^{-8}$.

^p $w_e y_e = +0.30_8$.

^q $\gamma_e = +0.0012_3$.

^r $H_0 = +0.46_3 \times 10^{-8}$.

^sFrom the value for In¹H and the predissociation in A ¹ Π .

^t $\Delta G(3/2) = 62.8$, $\Delta G(5/2) = 51.1$.

(continued on p. 349)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{115}\text{In}^{127}\text{I}$		$\mu = 60.303194$ $D_0^0 = 3.4_3 \text{ eV}^a$ I.P. = 8.50 eV^b Continuum with maximum at 31400 cm^{-1} .								JAN 1977
C 1Π								C \leftarrow X,		(1)
B $3\Pi_1$	25050.5	146.7	H 2.3					B \leftrightarrow X, R_V 25034.8	H ^Q	(1)*
A $3\Pi_0^+$	24401.6	158.5	H 1.7					A \leftrightarrow X, V_R 24392.0	H	(1)* (2)*
X $1\Sigma^+$	0	177.1	H 0.4	0.0368670	0.0001041 ₁ ^c	0.76	2.75365	Microwave sp. ^d		(3)(6)
$^{115}\text{In}^{127}\text{I}^+$		$D_0^0 = 0.7_2 \text{ eV}^e$ From the photoelectron spectrum (?).								JAN 1977
B ($^2\Sigma$)	(27300)									
A ($^2\Pi_{1/2}$)	(7700)									
A ($^2\Pi_{3/2}$)	(2300)									
X ($^2\Sigma$)	0									
$^{(115)}\text{In}^{160}$		$(\mu = 14.0404485)$ $2.9_4 \text{ eV} < D_0^0 \leq 3.2_5 \text{ eV}^a$								JAN 1977
A	23595.1	626.66	H 3.40	b				A \rightarrow X, R_V 23557.0	H	(1)*
(X $^2\Sigma$)	23033.1	703.09	H 3.71 ^c	b				22995.0	H	
$^{(115)}\text{In}^{(32)}\text{S}$		$(\mu = 25.0123666)$ $D_0^0 = 2.9_4 \text{ eV}^a$								JAN 1977
$^{(115)}\text{In}^{(121)}\text{Sb}$		$(\mu = 58.913758_3)$ $D_0^0 = 1.5_4 \text{ eV}^a$								JAN 1977
$^{(115)}\text{In}^{(80)}\text{Se}$		$(\mu = 47.134275_6)$ $D_0^0 = 2.5_0 \text{ eV}^a$								JAN 1977
$^{(115)}\text{In}^{(130)}\text{Te}$		$(\mu = 60.972685)$ $D_0^0 = 2.1_9 \text{ eV}^a$								JAN 1977

In¹H, In²H (continued):

^uΛ-type doubling, $\Delta v_{ef}(v=0) = + 0.0012 J(J+1)$. Breaking-off due to predissociation above $J'=13(v'=0,1)$, $10(v'=2)$, $7(v'=3)$.

^vB₁ = 1.098, B₂ = 0.981, B₃ = 0.751. D_v values have been determined (5) but their meaning is limited in view of the strong perturbations affecting this state. Fragments of three "extra" bands with $v''=0,1,2$.

^wΔG(3/2) = 857.42.

^xγ_e = - 0.0185.

- (1) Grundström, ZP 113, 721 (1939).
- (2) Garton, PPS A 64, 509 (1951).
- (3) Kleman, Dissertation (Stockholm, 1953).
- (4) Neuhaus, ZP 150, 4 (1958).
- (5) Neuhaus, ZP 152, 402 (1958).
- (6) Ginter, JMS 11, 301 (1963).
- (7) Larsson, Neuhaus, AF 27, 275 (1964).
- (8) Ginter, Battino, JCP 42, 3222 (1965).
- (9) Freed, JCP 45, 1714 (1966).
- (10) Ginter, JMS 20, 240 (1966).
- (11) Larsson, Neuhaus, Åslund, AF 37, 141 (1968).
- (12) Veseth, Lofthus, JMS 49, 414 (1974).
- (13) Veseth, JMS 59, 51 (1976).

InI, InI⁺:

^aBased on thermochemical data and spectroscopic evidence about the ¹Π and ³Π excited states; see (4).

Flame photometry gives 3.3₈ eV (5).

^bAdiabatic potential from the photoelectron spectrum (7); vertical potential 8.82 eV.

^cγ_e = + 8.0 × 10⁻⁸.

InI, InI⁺ (continued):

^dIndium and iodine quadrupole coupling constants (6).

^eFrom D₀⁰(InI) + I.P.(In) - I.P.(InI).

- (1) Wehrli, Miescher, HPA 6, 457 (1933); 7, 298 (1934).
- (2) Wehrli, HPA 7, 611, 676 (1934); 9, 587 (1936).
- (3) Barrett, Mandel, PR 109, 1572 (1958).
- (4) Barrow, TFS 56, 952 (1960).
- (5) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (6) Schenk, Tiemann, Hoeft, ZN 25 a, 1827 (1970).
- (7) Berkowitz, Dehmer, JCP 57, 3194 (1972).

InO: ^aThe lower limit is D₀⁰(InS); the upper limit, also based on mass-spectrometric evidence, was estimated by (3)(4).

^bA satisfactory interpretation of the observed bands is still lacking; see (1)(2). Preliminary rotational analysis of two bands by (5).

^cω_eγ_e = - 0.285.

- (1) Watson, Shambon, PR 50, 607 (1936).
- (2) Howell, PPS 57, 32 (1945).
- (3) Burns, De Maria, Drowart, Inghram, JCP 38, 1035 (1963).
- (4) Colin, Drowart, TFS 64, 2611 (1968).
- (5) Jacquinet, Lavendy, CR B 281, 397 (1975).

InS, InSe, InTe:

^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (4) of InO.

InSb: ^aThermochemical value (mass-spectrom.)(1).

(1) De Maria, Drowart, Inghram, JCP 31, 1076 (1959).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{127}\text{I}^{16}\text{O}$		$\mu = 14.2045833_3$ $D_0^0 = 1.8\text{ eV}^a$								JAN 1977
A $^2\Pi_{3/2}$	21557.8 ₁	514.5 ₇	Z 5.5 ₂	0.2763 ₅ ^b	0.0027 ₃	3.2	2.072 ₃	A \leftrightarrow X ₁ , ^c R 21474.0 ₅ Z		(1)* (2)* (3)*
X ₂ $^2\Pi_{1/2}$	(2330) ^d									
X ₁ $^2\Pi_{3/2}$	0	681.4 ₇	Z 4.2 ₉ ^e	0.34026 ^f	0.00269 ₆ ^g	3.6	1.8676	Microwave sp. ^h EPR sp.		(8) (5)(6)

IO: ^aBased on an extrapolation of the vibrational levels of A $^2\Pi_{3/2}$ and on the assumption that A dissociates into $^2P_{3/2} + ^1D$. Flame photometry (4) gives a value of 2.4 eV which seems less likely since it is as high as the value for BrO. The observed predissociation in A indicates $D_0^0 \leq 2.72$ eV. Extrapolation of the ground state gives 1.9₄ eV (7).

^bThe rotational lines of absorption bands with $v'=0$ and 2 are sharp; the lines of the 3-0 absorption band are distinctly diffuse, and the 1-0 and 4-0 bands are completely diffuse owing to predissociation (2).

^cFranck-Condon factors (9).

^dEstimated by (6) from spin-orbit coupling of component atoms.

^e $w_e y_e = -0.01_3$.

^fFrom the microwave spectrum (8) obtained $B_0(^2\Pi_{3/2}) = 0.338804$ which agrees well with the value from the electronic spectrum.

^g $\chi_e = -0.000009_7$.

^hMagnetic hyperfine interaction, nuclear quadrupole coupling constant.

- (1) Coleman, Gaydon, Vaidya, Nature 162, 108 (1948).
- (2) Durie, Ramsay, CJP 36, 35 (1958).
- (3) Durie, Legay, Ramsay, CJP 38, 444 (1960).
- (4) Phillips, Sugden, TFS 57, 914 (1961).
- (5) Carrington, Dyer, Levy, JCP 52, 309 (1970).
- (6) Brown, Byfleet, Howard, Russell, MP 23, 457 (1972).
- (7) Trivedi, Gohel, JP B 5, L38 (1972).
- (8) Saito, JMS 48, 530 (1973).
- (9) Rao, Rao, Rao, PL A 50, 341 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(^{193}\text{Ir}^{(11)}\text{B})$		$(\mu = 10.4150834) \quad D_0^0 = 5.2_7 \text{ eV}^a$							FEB 1975	
$(^{193}\text{Ir}^{12}\text{C})$		$(\mu = 11.29743405) \quad D_0^0 = 6.45 \text{ eV}^a$ Two unidentified bands at 15846 and 16504 cm^{-1} .							FEB 1975	
L $2\phi_{7/2}$	(20940)	(810)		[0.4812]		[6.8]	[1.760 ₉]	$L \leftrightarrow X_1$, R 20816.52 ^b Z	(3) (2)(3)	
K $2\pi_{3/2}$	19349	[832.7]	Z	0.5053	0.0051	7.4	1.718 ₄	$K \leftrightarrow X_1$, R 19236.64 ^b Z	(2)* (3)	
E ₂ $2\Delta_{3/2}$	$x_2 + (12180)$	(960)		0.5148	0.0043	[5.9] ^c	1.702 ₅	$E_2 \rightarrow X_2$, R 12145.3 ^d Z	(3)	
E ₁ $2\Delta_{5/2}$	15149.2	963.9	Z 5.4 ₄	0.5132	0.0040	6.2	1.705 ₂	$E_1 \leftrightarrow X_1$, R 15100.89 ^d Z	(3)*	
D $2\phi_{7/2}$	14413.5	935.7	Z 5.9 ₆	0.5053	0.0038	5.9	1.718 ₄	$D \leftrightarrow X_1$, R 14350.95 ^d Z	(3)*	
X ₂ $2\Delta_{3/2}$	x_2^e	(1030)		0.5272	0.0035	5.5	1.682 ₄			
X ₁ $2\Delta_{5/2}$	0	1060.1	Z 4.5 ₃	0.5268	0.0032	5.2	1.683 ₀			
$^{193}\text{Ir}^{16}\text{O}$		$\mu = 14.7705663 \quad D_0^0 = (3.6_4) \text{ eV}^a$ Additional bands at 14338, 14490 cm^{-1} (2), and 17070 cm^{-1} (2)(4).							FEB 1975	
H' (3/2)				[0.3378] ^b		[4.0] ^b	[1.838 ₁]	$H' \rightarrow A'$, R 22005.8 ^{cb} Z	(2)(4) (4)	
H'' 5/2		d		[0.3371]	d	[4.0]	[1.840 ₀]	$H'' \rightarrow A''$, R 21869.7 ^c Z	(4)	
D (3/2)	$a' + 17720$	[672.5]	Z	0.3534 ^e	0.0026	[3.2]	1.797 ₁	$D \rightarrow A'$, R 17602.72 ^c Z	(4)*	
A'' 5/2 ^f		903.3	Z 4.7	0.3867 ^g	0.0024	[2.9]	1.718 ₀			
A' (3/2) ^f	a'	909.4	Z 4.7	0.3847	0.0025	3.0	1.722 ₄			
$(^{193}\text{Ir}^{(28)}\text{Si})$		$(\mu = 24.434297_5) \quad D_0^0 = 4.7_6 \text{ eV}^a$							FEB 1975	
$(^{193}\text{Ir}^{232}\text{Th})$		$(\mu = 105.352106) \quad D_0^0 = 5.9 \text{ eV}^a$							FEB 1975	

IrB: ^aThermochemical value (mass-spectrom.)(1).

(1) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart, TFS 66, 809 (1970).

IrC: ^aThermochemical value (mass-spectrom.)(1)(4).

^bJ'=0 relative to J''=0, calculated from the data in (3).

^cD₁ = 5.4×10^{-7} .

^dJ'=0 relative to J''=0. A different definition of the band origins is used in (3).

^ex₂ ≈ 3200 cm⁻¹; see (3).

(1) McIntyre, Vander Auwera-Mahieu, Drowart, TFS 64, 3006 (1968).

(2) Jansson, Scullman, Yttermo, CPL 4, 188 (1969).

(3) Jansson, Scullman, JMS 36, 248 (1970).

(4) Gingerich, CPL 23, 270 (1973).

IrO: ^aThermochemical value, estimated (3) from mass-spectrometric results of (1).

^bOnly one perturbed vibrational level of H' analyzed; vibrational numbering uncertain.

^cJ'=0 relative to J''=0.

^dThree additional levels, numbered I, II, and III by (4), have been identified in transitions to A" and may represent v=1, 2, and 3 of H". With this interpretation B₁, ..., B₃ = 0.3307, 0.326, 0.3205, and ΔG(1/2, ..., 3/2) = 605.2 Z, 564.6, 544.3.

^ePerturbation in v=0 at J=59½.

^fA' and A" may be the two components of a ²Δ state.

^gPerturbations.

(1) Norman, Staley, Bell, JCP 42, 1123 (1965).

(2) Raziunas, Macur, Katz, JCP 43, 1010 (1965).

(3) Drowart, Goldfinger, AC (Int. Ed. Engl.) 6, 581 (1967).

(4) Jansson, Scullman, JMS 43, 208 (1972).

IrSi: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (1) of IrB.

IrTh: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (4) of IrC.

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{39}\text{K}_2$		$\mu = 19.4818545$ $D_0^0 = 0.514 \text{ eV}^a$ I.P. = 4.0 eV^b Unidentified diffuse emission bands, $17460 - 17840 \text{ cm}^{-1}$. Diffuse bands close to lines of the principal series of K; fragments of additional systems.								JAN 1977 A	
G	28091	64.9_0^c	H 0.55					G \leftarrow X, R 28077	H	(24)	
F	27571	62.2_9^c	H 0.2 ₄					F \leftarrow X, R 27556	H	(5)(7)(8)	
E	26494.0	61.8^d	H 0.2 ₈					E \leftarrow X, R 26478.9	H	(10)	
D	24627.7	61.60	H 0.90 ^e					D \leftarrow X, R 24612.3	H	(10)(13)	
C	$^1\Pi_u$ 22969.4 ₃	61.48_5	Z 0.13 ₃	0.04404	0.00011 ^f		4.433	C \leftarrow X, R 22954.2 ₀	Z	(12)	
B	$^1\Pi_u$ 15376.7 ₄	75.00	0.3876 ^g	0.04876_3^h	0.00024	8.2 ₅	4.212 ₅	B ⁱ \leftrightarrow X, ^j R 15368.2 ₀	Z	(1)(12)(15)	
A	$^1\Sigma_u^+$ 11681.9	69.09	H 0.153	k				A \leftrightarrow X, R 11670.5	H	(4)(6)(20)	
a	$^3\Sigma_u^+$	Not observed; scattering calculations predict a very shallow potential minimum at $\sim 8.7 \text{ \AA}$.									(2)(25)
X	$^1\Sigma_g^+$ 0	92.021	Z 0.2829 ^l	0.056743	0.000165 ^m	8.63	3.9051	Mol. beam magn. reson. ⁿ		(27)	
$(^{39})\text{K}_2^+$		$D_0^0 = 0.8_5 \text{ eV}^o$								JAN 1977	
X $^2\Sigma_g^+$ 0		No spectrum observed. The formation of K(4p) in (K^+, K) collisions has been studied by (28) who have interpreted the magnitude and velocity dependence of the cross section in terms of properties of the potential curves for the lowest excited states of K_2^+ . (67) ^p								(4.11) ^p	
$^{39}\text{K}^{40}\text{Ar}$		$\mu = 19.7283641$ $D_0^0 = 0.0053 \text{ eV}^a$ Predicted potential energy curves for higher excited states (6). { Continuous emission with maximum at 19672 cm^{-1} , shifted by 1355 cm^{-1} from the forbidden K 5s-4s line at 21027 cm^{-1} . Theoretical interatomic potentials (3).								JAN 1977	
C	$^2\Sigma$							C \rightarrow X,		(10)	
A	$^2\Pi$, B $^2\Sigma$										
X	$^2\Sigma^+$ 0							5.2 ^a	Mol. beam magn. reson. ^b	(4)(5)(9)	

K_2, K_2^+ :

^aFrom the convergence limit of $B^1\Pi_u$. Thermochemical value [(3), recalcd. (6)] 0.56 eV.

^bPhotoionization of K_2 (21); in agreement with limits (3.57 < I.P. < 4.11 eV) obtained from chemi-ionization thresholds (17)(19). (15) estimate 4.09 eV.

^cAnalysis by (10); not confirmed by (13).

^dAverage of the constants obtained by (10)(13).

^e $w_e y_e = + 0.0010, w_e z_e = - 0.00030$; convergence at 25590.

^f $y_e = + 3 \times 10^{-6}$.

^g $w_e y_e = + 0.004366, w_e z_e = - 0.0001830$; vibrational constants for $v' < 25$ from low-resolution magnetic rotation spectra. Higher vibrational levels converge rapidly at 17160 cm^{-1} above $X^1\Sigma_g^+, v=0$. T_e is from the analysis of high-resolution laser-induced fluorescence spectra (20).

^hRecalculated by (20) from the data of (4).

ⁱRadiative lifetime $\tau(v=6,7,8) = 12.4 \text{ ns}$ (23);

(22) measured 9.7 ns.

^jAbsorption cross sections (18).

^kA complex magnetic rotation spectrum has been observed which may be due to perturbations of $A^1\Sigma_u^+$ by an unidentified $^3\Pi$ state (9).

^l $w_e y_e = - 0.002055$. Vibrational and rotational constants from the laser-induced $B \rightarrow X$ fluorescence spectrum (20).

^m $-7.2 \times 10^{-6}(v+\frac{1}{2})^2 + 1.5 \times 10^{-7}(v+\frac{1}{2})^3$. See ^l.

ⁿ $g_J = 0.02163 \mu_N$ (16). For NMR spectrum and potassium eqQ see (11)(14).

^oFrom $D_0^0(K_2) + \text{I.P.}(K) - \text{I.P.}(K_2)$. The experimentally observed limits (photoionization of potassium vapour) are $0.74 \text{ eV} < D_0^0 < 1.27 \text{ eV}$ (19). Theoretical calculations (26) give 1 eV.

^pTheoretical calculations (26).

(1) Yamamoto (1929), revised by (2).

K_2, K_2^+ (continued):

(2) Crane, Christy, PR 36, 421 (1930).

(3) Lewis, ZP 69, 786 (1931).

(4) Loomis, PR 38, 2153 (1931).

(5) Kuhn, ZP 76, 782 (1932).

(6) Loomis, Nusbaum, PR 39, 89 (1932).

(7) Chakraborti, IJP 10, 155 (1935).

(8) Okuda, Nature 138, 168 (1936).

(9) Carroll, PR 52, 822 (1937).

(10) Yoshinaga, PPMSJ 19, 847, 1073 (1937).

(11) Kusch, Millman, Rabi, PR 55, 1176 (1939).

(12) Sinha, PPS 60, 436 (1948).

(13) Sinha, PPS A 63, 952 (1950).

(14) Logan, Cote, Kusch, PR 86, 280 (1952).

(15) Robertson, Barrow, PCS (1961), 329.

(16) Brooks, Anderson, Ramsey, PRL 10, 441 (1963); PR A 136, 62 (1964).

(17) Lee, Mahan, JCP 42, 2893 (1965).

(18) Lapp, Harris, JQSRT 6, 169 (1966).

(19) Williams, JCP 47, 4281 (1967).

(20) Tango, Link, Zare, JCP 49, 4264 (1968).

(21) Foster, Leckenby, Robbins, JP B 2, 478 (1969).

(22) Baumgartner, Demtröder, Stock, ZP 232, 462 (1970).

(23) Tango, Zare, JCP 53, 3094 (1970).

(24) Rebbeck, Vaughan, JP B 4, 258 (1971).

(25) Sorokin, Lankard, JCP 55, 3810 (1971).

(26) Bellomonte, Cavaliere, Ferrante, JCP 61, 3225 (1974).

(27) Geittner, ZP A 272, 359 (1975).

(28) Aquilanti, Casavecchia, JCP 64, 751 (1976).

KAR, KAR^+ : see p. 357.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(39) $K^{40}Ar^+$ X $1\Sigma^+$				$D_e^0 = 0.12_2 \text{ eV}^c$			2.8_8^c			JAN 1977 A
(39) $K^{79}Br$ A X $1\Sigma^+$	0			$\mu = 26.0849820$ $D_0^0 = 3.91 \text{ eV}^a$ Two peaks in the electron energy loss spectrum at 19.7 and 23.7 eV (13) may be associated with excitation of an electron from the metal 3p shell of K^+Br^- . Continuous absorption above 31000 cm^{-1} , maxima at 36000, 39300, 47600 cm^{-1} . ^c Diffuse absorption bands, $25000 - 31000 \text{ cm}^{-1}$. ^d The chemiluminescence spectrum (gas - beam, or flame) consists of a long ground-state vibrational progression stretching from 17500 to 31500 cm^{-1} , the onsets and cutoffs depending on the prevailing conditions of the experiment. ^d				$A \leftrightarrow X$		JAN 1977 (1)(4) (2)(3)(4)(5) (15)(16) (7) (6)(10) (12)(14)
				213^e (0.80)	0.08122109	0.00040481^f	4.461_9^g	2.82078	Rotation-vibration sp. Rotation sp. Mol. beam rf el. reson. ^h	
(39) $K(79)Br^+$ D ($\frac{1}{2}$) (137300) ^j C ($\frac{3}{2}, \frac{1}{2}$) 134700 ^j A ($\frac{1}{2}$) 3900 ^j X ($\frac{3}{2}, \frac{1}{2}$) 0 ^j				$D_0^0 = 0.4_0 \text{ eV}^i$ Removal of an electron from the metal 3p shell. Removal of an electron from the halogen 4p shell.						JAN 1977

KAr, KAr⁺:

^aBased on atomic scattering data (1)(2)(8). The ground state potential supports nine vibrational levels (9).

^bThe spin-rotation interaction [$\gamma(v=0) = 8.0 \times 10^{-6}$] (4)(9) as well as the hyperfine interaction (5) have been investigated.

^cFrom K⁺-off-Ar total scattering cross sections (7); references to earlier experimental and theoretical work may be found in this paper.

- (1) Buck, Pauly, ZP 208, 390 (1968).
- (2) Düren, Raabe, Schlier, ZP 214, 410 (1968).
- (3) Baylis, JCP 51, 2665 (1969).
- (4) Mattison, Pritchard, Kleppner, PRL 32, 507 (1974).
- (5) Freeman, Mattison, Pritchard, Kleppner, PRL 33, 397 (1974).
- (6) Pascale, Vandeplanque, JCP 60, 2278 (1974).
- (7) Budenholzer, Galante, Gislason, Jorgensen, CPL 33, 245 (1975).
- (8) Fluendy, Kerr, Lawley, McCall, JP B 8, L190 (1975).
- (9) Freeman, Mattison, Pritchard, Kleppner, JCP 64, 1194 (1976).
- (10) Tam, Moe, Bulos, Happer, OC 16, 376 (1976).

KBr, KBr⁺:

^aThermochemical value (8)(9); from the analysis of the fluctuation bands in the UV absorption spectrum (4) and (5) estimate 3.96 and ± 4.10 eV, respectively.

^bAdiabatic potential from the photoelectron spectrum (17), not corrected for thermal population of the ground state vibrational levels; vertical potential 8.34 eV.

^cAbsorption cross sections (11). The electron energy loss spectrum (13) has peaks at 37000, 52000, 63000 cm⁻¹.

KBr, KBr⁺ (continued):

^dSee ^d of CsBr. From the emission data (16) have constructed a tentative upper-state potential energy curve which is, however, dependent on the model potential used for the ground state.

^eFrom the IR spectrum. The Dunham theory applied to the microwave results gives $\omega_e = 219.17$, $\omega_e x_e = 0.758$ (10).

^f $\gamma_e = + 7.7 \times 10^{-7}$.

^g $\beta_e = - 0.0002 \times 10^{-8}$.

^h $\mu_{el}[D] = 10.60256 + 0.0504_5(v+\frac{1}{2}) + 0.00015(v+\frac{1}{2})^2$ (12)(14); nuclear quadrupole and spin-rotation constants in (14), see also (6).

ⁱFrom D₀⁰(KBr) + I.P.(K) - I.P.(KBr); (17) give 0.33 eV.

^jFrom the maxima of the photoelectron spectrum (17)(18).

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Beutler, Josephy, ZP 53, 747 (1929).
- (3) Sommermeyer, ZP 56, 548 (1929).
- (4) Levi, Dissertation (Berlin, 1934).
- (5) Barrow, Caunt, PRS A 219, 120 (1953).
- (6) Fabricand, Carlson, Lee, Rabi, PR 91, 1403 (1953).
- (7) Rice, Klemperer, JCP 27, 573 (1957).
- (8) Brewer, Brackett, CRev 61, 425 (1961).
- (9) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (10) Rusk, Gordy, PR 127, 817 (1962).
- (11) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (12) van Wachem, de Leeuw, Dymanus, JCP 47, 2256 (1967).
- (13) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (14) de Leeuw, van Wachem, Dymanus, JCP 50, 1393 (1969).
- (15) Oldenborg, Gole, Zare, JCP 60, 4032 (1974).
- (16) Kaufmann, Kinsey, Palmer, Tewarson, JCP 61, 1865 (1974).
- (17) Potts, Williams, Price, PRS A 341, 147 (1974).
- (18) Potts, Williams, JCS FT II 72, 1892 (1976).

KCl, KCl⁺:

- ^aThermochemical value (8)(9); the analysis of the fluctuation bands gave $D_0^0 = 4.39$ eV (and $w'' = 280$) according to (3) or $D_0^0 \leq 4.66$ eV (and $w'' = 305$) according to (4).
- ^bAdiabatic potential from the photoelectron spectrum of (17), not corrected for thermal population of ground state vibrational levels; the band maximum (vertical potential) is at 8.92 eV.
- ^cUV absorption cross sections (11). In the electron energy loss spectrum (13) there are peaks at 42000, 53000, and 68000 cm⁻¹.
- ^dSee ^d of CsBr. From the emission data (16) have derived a tentative potential energy curve for the upper state (see ^d of KBr); $D_e' \approx 450$ cm⁻¹.
- ^eFrom the IR spectrum. The Dunham theory applied to the microwave results gives $w_e = 279.8_0$, $w_e x_e = 1.167$.
- ^f $r_e = + 1.6_3 \times 10^{-6}$.
- ^g $\beta_e = - 8.3 \times 10^{-11}$.
- ^hIR study of matrix isolated KCl (18).
- ⁱ $\mu_{el}[D] = 10.239_1 + 0.0596_8(v+\frac{1}{2}) + 0.00019(v+\frac{1}{2})^2$ (12)(14); nuclear electric quadrupole and spin-rotation coupling constants (12).
- ^jFrom $D_0^0(KCl) + I.P.(K) - I.P.(KCl)$; (17) give 0.19 eV.
- ^kFrom the maxima in the photoelectron spectrum (17)(19). The two peaks corresponding to the $^2P_{3/2}$ and $^2P_{1/2}$ components of normal Cl are not resolved.

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Beutler, Josephy, ZP 53, 747 (1929).
- (3) Levi, Dissertation (Berlin, 1934).
- (4) Barrow, Caunt, PRS A 219, 120 (1953).
- (5) Lee, Fabricand, Carlson, Rabi, PR 91, 1395 (1953).

KCl, KCl⁺ (continued):

- (6) Tate, Strandberg, JCP 22, 1380 (1954).
- (7) Rice, Klemperer, JCP 27, 573 (1957).
- (8) Brewer, Brackett, CRev 61, 425 (1961).
- (9) Bulewicz, Phillips, Sugden, TFS 52, 921 (1961).
- (10) Clouser, Gordy, PR A 134, 863 (1964).
- (11) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (12) van Wachem, Dymanus, JCP 46, 3749 (1967).
- (13) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (14) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
- (15) Oldenberg, Gole, Zare, JCP 60, 4032 (1974).
- (16) Kaufmann, Kinsey, Palmer, Tewarson, JCP 61, 1865 (1974).
- (17) Potts, Williams, Price, PRS A 341, 147 (1974).
- (18) Ismail, Hauge, Margrave, JMS 54, 402 (1975).
- (19) Potts, Williams, JCS FT II 72, 1892 (1976).

KCs: ^aInterpolated values based on the constants for K₂ and Cs₂ (2).

- (1) Walter, Barratt, PRS A 119, 257 (1928).
- (2) Cavaliere, Ferrante, Lo Cascio, JCP 62, 4753 (1975).

KF: ^aThermochemical value (6)(7); an upper limit, $D_0^0 \leq 5.28$ eV, was derived (3) from the analysis of the fluctuation bands.

(continued on p. 361)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{39}\text{K}^{19}\text{F}$ (continued)										
A		Fluctuation bands, 34300 - 46700 cm^{-1} (absorption).						A \leftarrow X	(3)	
X $1\Sigma^+$	0	428 ^b	(2.4)	0.27993741 ₃	2.33503 ₈ ^c $\times 10^{-3}$	0.04834 ^d	2.17145 ₇	Rot.-vibr. sp. ^e Rotation sp. Mol. beam rf electric ^f and magn. reson. ^g	(9)(12) (2)(5)(10) (17) (13)(14)(15) (11)	
$^{39}\text{K}^1\text{H}$										
		$\mu = 0.98241434$ $D_0^0 = (1.8_6) \text{ eV}$ [extrapol. of A 1Σ]							JAN 1977	
		Theoretical potential energy curves, coupling between molecular states (8).								
		Fluctuating continuum in emission, 25000 - 33000 cm^{-1} .							(3)	
A $1\Sigma^+$	19052.8	228.2	Z	-5.7 ₅ ^a	1.26 ₉	-0.037 ₅ ^b	9.5	3.68	A ^c \leftrightarrow X, R 18680.1	Z (1)(2)(5)(6)
X $1\Sigma^+$	0	983.6	Z	14.3 ₂	3.412 ₃	0.081 ₇	15.3	2.242 ₅		
$^{39}\text{K}^2\text{H}$										
		$\mu = 1.91510699$ $D_0^0 = (1.8_9) \text{ eV}$							JAN 1977	
A $1\Sigma^+$	19060	161	Z	-3.3 ^d	0.65 ₉	-0.012 ₇ ^e	2.7	3.65	A \leftrightarrow X, R 18790	Z (4)(6)
X $1\Sigma^+$	0	706.6	Z	7.7 ₃	1.753 ₉	0.0318	4.7	2.240 ₃		
$^{39}\text{K}^{127}\text{I}$										
		$\mu = 29.8108348$ $D_0^0 = 3.31 \text{ eV}^a$ I.P. = 7.2 ₁ eV^b							JAN 1977	
		Features in the electron energy loss spectrum (12)(22) at $\sim 3.8, 4.7, 5.1 \text{ eV}$ correspond to maxima in the absorption spectrum. Peaks at higher energies could indicate that KI absorbs strongly in the VUV region; structure above 19 eV may arise from excitation of a metal 3p electron.								
		Continuous absorption ^c above 26500 cm^{-1} , maxima at 30800, 38400, 41700 ^d cm^{-1} .							(1)(4)(11)	

KF (continued):

^bFrom the IR spectrum (9)(12). (10), applying the Dunham theory to the microwave results, calculate $\omega_e = 426.0_4$

and $\omega_e x_e = 2.4_3$.

^c $\gamma_e = + 6.96_3 \times 10^{-6}$.

^d $\beta_e = - 2 \times 10^{-10}$.

^eIR spectrum of matrix isolated KF (18).

^f $\mu_{el}[D] = 8.5583 + 0.06841(v+\frac{1}{2}) + 0.000256(v+\frac{1}{2})^2$ (8)(15), electric quadrupole and other hyperfine coupling constants (4)(13)(14); see also (2)(5).

^g $g_J = (-)0.036_4 \mu_N$ (11).

(1) Müller, AP(Leipzig) 82, 39 (1927).

(2) Grabner, Hughes, PR 79, 819 (1950).

(3) Barrow, Caunt, PRS A 219, 120 (1953).

(4) Schlier, ZP 147, 600 (1957).

(5) Green, Lew, CJP 38, 482 (1960).

(6) Brewer, Brackett, CREV 61, 425 (1961).

(7) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(8) Gräff, Runolfsson, ZP 176, 90 (1963).

(9) Ritchie, Lew, CJP 42, 43 (1964).

(10) Veazey, Gordy, PR A 138, 1303 (1965).

(11) Mehran, Brooks, Ramsey, PR 141, 93 (1966).

(12) Baikov, Vasilevskii, OS(Engl. Transl.) 22, 198 (1967).

(13) Bonczyk, Hughes, PR 161, 15 (1967).

(14) van Wachem, Dymanus, JCP 46, 3749 (1967).

(15) van Wachem, de Leeuw, Dymanus, JCP 47, 2256 (1967).

(16) Geiger, Pfeiffer, ZP 208, 105 (1968).

(17) Dijkerman, Flegel, Gräff, Mönster, ZN 27 a, 100 (1972).

(18) Ismail, Hauge, Margrave, JINC 35, 3201 (1973).

K^1H , K^2H :

^a $\omega_e y_e = - 0.169$. The $\Delta G(v+\frac{1}{2})$ curve has a maximum at $v \approx 11$.

^b $\gamma_e = - 0.0023_2$. The B_v curve has a maximum at $v \approx 7$.

^cRadiative lifetime $\tau < 10$ ns (7).

^d $\omega_e y_e = - 0.07_2$. The $\Delta G(v+\frac{1}{2})$ curve has a maximum at $v \approx 16$.

^e $\gamma_e = - 0.0005_7$. The B_v curve has a maximum at $v \approx 11$.

(1) Almy, Hause, PR 42, 242 (1932).

(2) Hori, Mem. Ryojun Coll. Engng. 6, 1 (1933).

(3) Hori, Mem. Ryojun Coll. Engng. 6, 115 (1933).

(4) Imanishi, Sci. Pap. IPCR (Tokyo) 39, 45 (1941).

(5) Almy, Beiler, PR 61, 476 (1942).

(6) Bartky, JMS 20, 299 (1966).

(7) Cruse, Zare, JCP 60, 1182 (1974).

(8) Numrich, Truhlar, JPC 79, 2745 (1975).

KI: ^aThermochemical value (8); flame photometry (9) gives 3.4_9 eV. Earlier spectroscopic estimates were 3.31 eV (4) and ≤ 3.47 eV (6).

^bAdiabatic potential from the photoelectron spectrum (19), not corrected for thermal population of ground state vibrational levels; band maximum (vertical potential) at 7.68 eV.

^cAbsorption cross sections (11). A preliminary measurement of the photodissociation product anisotropy by photofragment spectroscopy at 28800 cm^{-1} (18) indicates strong contributions from perpendicular transitions.

^dPhotodissociation produces $K(4p^2P)$; similarly, photodissociation at 52600 cm^{-1} leads to $K(5p^2P)$ (17).

(continued on p. 363)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{39}\text{K}^{127}\text{I}$ (continued)										
A (0^+)	(26620)	This is one of five very shallow states ($0^+, 0^-, 1, 1, 2$) ^e arising from normal atomic products $\text{K}(^2\text{S}_{1/2}) + \text{I}(^2\text{P}_{3/2})$. The analysis of K-off-I differential elastic scattering measurements (14) suggests that only 0^+ ($D_e \approx 150 \text{ cm}^{-1}$, $r_e \approx 3.85 \text{ \AA}$) is favorably situated for transitions from the ground state. Accordingly, (15) have analyzed the fluctuation bands observed in absorption from 19600 to 27000 cm^{-1} (3)(4) and in chemiluminescence ^f from 16300 to 26200 cm^{-1} (4)(15)(16) in terms of the $\text{A} \leftrightarrow \text{X}$ transition, assigning vibrational quantum numbers v'' from 2 to 64, and constructing an accurate potential curve for the excited state.								
X $1\Sigma^+$	0	186.53 ^g	0.574	0.06087473	0.00026776 ^h	2.593 ₄ ⁱ	3.04784 ₄	Rotation spectrum ^j		(7)(10)
$(^{39})\text{K}^{127}\text{I}^+$										
D ($\frac{1}{2}$)	(143700) ^l	$D_0^0 = 0.4_4 \text{ eV}^k$								
C ($\frac{3}{2}, \frac{1}{2}$)	140800 ^l									
A ($\frac{1}{2}$)	7900 ^l	Removal of an electron from the halogen 5p shell.								
X ($\frac{3}{2}, \frac{1}{2}$)	0 ^l									
$(^{39})\text{K}(^{84})\text{Kr}$										
C 2Σ		($\mu = 26.6083236$)	$D_e^0 = 0.0089 \text{ eV}^a$	Continuous emission with maximum at 19530 cm^{-1} , shifted by 1497 cm^{-1} from the forbidden K 5s-4s line at 21027 cm^{-1} .				C \rightarrow X		JAN 1977
B 2Σ	}	Theoretical interatomic potentials (3).								
A 2Π										
X $2\Sigma^+$										
							5.1 ^a			(4)

KI, KI⁺ (continued):

^eA differential scattering experiment investigating the collisional depolarization of polarized K atoms (20) leads to the conclusion that J,J coupling would provide the most adequate description of these states.

^fThe actual onset and cutoff wavelengths depend on the experimental conditions: a beam-gas arrangement (16) or flames (4)(15).

^gFrom the microwave results by use of Dunham's theory.

^h $r_e = + 3.88 \times 10^{-7}$.

ⁱ $A_e = + 4 \times 10^{-12}$.

^jQuadrupole hyperfine structure (13). The dipole moment $\mu_{el} = 10.82$ D was measured by the electric deflection method (23); see also (5).

^kFrom $D_0^0(KI) + I.P.(K) - I.P.(KI)$; (19) give 0.37 eV.

^lFrom band maxima of the photoelectron spectrum (19)(21).

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Beutler, Josephy, ZP 53, 747 (1929).
- (3) Sommermeyer, ZP 56, 548 (1929).
- (4) Levi, Dissertation (Berlin, 1934).
- (5) Rodebush, Murray, Bixler, JCP 4, 372 (1936).
- (6) Barrow, Caunt, PRS A 219, 120 (1953).
- (7) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (8) Brewer, Brackett, CRev 61, 425 (1961).
- (9) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (10) Rusk, Gordy, PR 127, 817 (1962).

KI, KI⁺ (continued):

- (11) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (12) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (13) Tiemann, El Ali, Hoeft, Törring, ZN 28 a, 1058 (1973).
- (14) Kaufmann, Lawter, Kinsey, JCP 60, 4016 (1974).
- (15) Kaufmann, Kinsey, Palmer, Tewarson, JCP 60, 4023 (1974).
- (16) Oldenborg, Gole, Zare, JCP 60, 4032 (1974).
- (17) Earl, Herm, JCP 60, 4568 (1974).
- (18) Ormerod, Powers, Rose, JCP 60, 5109 (1974).
- (19) Potts, Williams, Price, PRS A 341, 147 (1974).
- (20) Carter, Pritchard, JCP 62, 927 (1975).
- (21) Potts, Williams, JCS FT II 72, 1892 (1976).
- (22) Rudge, Trajmar, Williams, PR A 13, 2074 (1976).
- (23) Story, Hebert, JCP 64, 855 (1976).

KKr: ^aFrom atomic scattering data (1)(2)

- (1) Buck, Pauly, ZP 208, 390 (1968).
- (2) Düren, Raabe, Schlier, ZP 214, 410 (1968).
- (3) Baylis, JCP 51, 2665 (1969).
- (4) Tam, Moe, Bulos, Happer, OC 16, 376 (1976).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(39)K ¹⁶ O		$(\mu = 11.3398256_4)$								JAN 1977
A 2_{Π}	(347) ^a	(442) ^a					(2.33) ^a			
X 2_{Σ}^+	0 ^a	(384) ^b					(2.22) ^a			
(39)K ¹⁶ O ⁺		$D_0^0(K^+-O) = 0.2 \text{ eV}^c$								JAN 1977
(84)Kr ₂		$(\mu = 41.955752_7)$ $D_0^0 = 0.0157 \text{ eV}^a$ I.P. = 12.87 eV ^b								APR 1977 A
		Several emission continua in the near infrared, visible, and ultra-violet; interpretation doubtful.								(2)(11)
		Four unclassified band systems, 92530 - 94200 cm ⁻¹ ; the upper states are probably derived from the configuration $4p^6 1s + 4p^5(^2P_{\frac{3}{2}})5p$.								(7)
D (1_u)	(86000)	Probably a repulsive state; several diffuse bands shortward of the second resonance line (upper state $5s'[\frac{1}{2}]1_u$) at 1165 \AA (85848 cm ⁻¹).						$D \leftrightarrow X$,		(7)*
C (0_u^+)	85522.0	43.3 ₁	H	1.74	Band system converging to $1s + 5s'[\frac{1}{2}]1_u$; $v'' = 0 \dots 9$, $v' = 0 \dots 5$.		$C \leftarrow X$, $v = 85531.5$	H	(7)*	
		Additional unclassified absorption bands shortward of the first resonance line (upper state $5s[\frac{3}{2}]1_u$) at 1236 \AA (80918 cm ⁻¹); 80927 - 81001 cm ⁻¹ .								(7)
B (0_u^+)	(80006)	[80.8] ^c	H	Band system converging to $1s + 5s[\frac{3}{2}]1_u$; $v'' = 0 \dots 9$, $v' = (0 \dots 12)^c$.		$B \leftarrow X$, $v = 80035^c$	H	(7)*		
A (1_u)	(79613)	[67.3] ^c	H	Band system converging to $1s + 5s[\frac{3}{2}]2_u$; $v'' = 1 \dots 7$, $v' = (0 \dots 5)^c$.		$A \leftarrow X$, ^d $v = 79635^c$	H	(7)*		
		Continuous emission with two maxima usually referred to as the "first continuum" closer to the first resonance line at 1236 \AA (80918 cm ⁻¹) and the "second continuum" at 1470 \AA (68000 cm ⁻¹).						$A, B \rightarrow X$, ^e	(1)*	
X $1_{\Sigma_g}^+$	0	24.1 ₈	H	1.34 ^f			4.0 ₃ ^g			
(84)Kr ₂ ⁺		$(\mu = 41.955615_5)$ $D_0^0 = 1.15 \text{ eV}^h$								APR 1977 A
		Some excited states have been qualitatively discussed by (10a).								
X ($2_{\Sigma_u}^+$)	0							(2.6) [estimated value (9a)]		

KO, KO^+ :

^aAb initio calculation by (4). The relative position of the two states is in accordance with results of a magnetic deflection analysis of $\text{M} + \text{NO}_2$ scattering products (M = alkali metal) by (1).

^bFundamental in solid nitrogen matrix (2); the ab initio value is $\omega_e = 467 \text{ cm}^{-1}$ (4).

^cFrom a merging beam study of the reaction $\text{CO}^+(\text{K,C})\text{KO}^+$ (3).

(1) Herm, Herschbach, JCP 52, 5783 (1970).

(2) Spiker, Andrews, JCP 58, 713 (1973).

(3) Rol, Entemann, Wendell, JCP 61, 2050 (1974).

(4) So, Richards, CPL 32, 227 (1975).

Kr_2 , Kr_2^+ :

^aFrom the absorption spectrum (7). Various other methods, reviewed in (7), agree well with the spectroscopic value; see also ^g.

^bFrom photoionization studies (14); see also the earlier work of (3)(4).

^cThe v' numbering assumes that the lowest observed level has $v'=0$ which may, however, not be the case.

^dA fairly strong diffuse R shaded band (called "spectral demarcation") at 79923 cm^{-1} is considered to belong to the same electronic transition (7).

^eThe emission is attributed to transitions from the lowest excited states $\text{A } ^3\Sigma_u^+(1_u)$ and $\text{B } ^1\Sigma_u^+(0_u^+)$ to the repulsive part of the ground state potential; for a detailed discussion of the analogous spectrum of Xe_2 see (4a). The "second continuum" was recently observed in emission from high-pressure krypton excited by high-current short-duration electron bursts from a Febetron source (12) and was found to be characterized by three radiative decay con-

Kr_2 , Kr_2^+ (continued):

stants of 9, 32, 350 ns. Similar excitation (10) produces "long-lived" ($\tau = 353 \text{ ns}$) molecular species which absorb at 10100, 10160, 10250, 10350 cm^{-1} . The 1470 Å emission was also observed from Kr_2 in a neon matrix excited by α particles (6).

^f $\omega_e y_e = +0.022$; vibrational levels observed to $v=9$.

^gFrom viscosity data, virial coefficients (9) and collision cross sections (5). More recently, (8) have derived $r_e = 4.007 \text{ Å}$ and $D_e = 0.0174 \text{ eV}$ from a combination of all available data; see also (13).

^h $D_0^0(\text{Kr}_2) + \text{I.P.}(\text{Kr}) - \text{I.P.}(\text{Kr}_2)$. From elastic scattering of Kr^+ by Kr (9a) obtain $D_e = 1.21 \text{ eV}$.

(1) Tanaka, JOSA 45, 710 (1955).

(2) Herman, Herman, Nature 195, 1086 (1962).

(3) Huffman, Katayama, JCP 45, 138 (1966).

(4) Samson, Cairns, JOSA 56, 1140 (1966).

(4a) Mulliken, JCP 52, 5170 (1970).

(5) Buck, Dondi, Valbusa, Klein, Scoles, PR A 8, 2409 (1973).

(6) Gedanken, Raz, Jortner, JCP 59, 1630 (1973).

(7) Tanaka, Yoshino, Freeman, JCP 59, 5160 (1973).

(8) Barker, Watts, Lee, Schafer, Lee, JCP 61, 3081 (1974).

(9) Gough, Smith, Maitland, MP 27, 867 (1974).

(9a) Mittmann, Weise, ZN 29 a, 400 (1974).

(10) Oka, Rao, Redpath, Firestone, JCP 61, 4740 (1974).

(10a) Barr, Dee, Gilmore, JQSRT 15, 625 (1975).

(11) Birot, Brunet, Galy, Millet, Teyssier, JCP 63, 1469 (1975).

(12) Koehler, Ferderber, Redhead, Ebert, PR A 12, 968 (1975).

(13) Nain, Aziz, Jain, Saxena, JCP 65, 3242 (1976).

(14) Ng, Trevor, Mahan, Lee, JCP 66, 446 (1977).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(39)K(85)Rb X $1\Sigma^+$		($\mu = 26.7080933$) Diffuse absorption band at 20160 cm $^{-1}$. (75.5) ^a					(4.07) ^a			JAN 1977 (1)
(84)Kr(79)Br B (48130) X 0		($\mu = 40.669180_4$) (166) Broad diffuse peaks, principal peak at 48440 cm $^{-1}$. ^a Repulsive state with rather flat potential function.						B \rightarrow X,		APR 1977 (1)
(84)Kr(35)Cl D B (44890) X 0		($\mu = 24.6827076$) (210) Broad diffuse peaks, principal peak at 45350 cm $^{-1}$. ^a Repulsive state with very flat potential function.						D \rightarrow X, B \rightarrow X,	50250 45040	APR 1977 (2) (1)(2)
(84)Kr $19F$ E (2Σ) (71500) ^a D (2Π) $\frac{1}{2}$ (48000) ^a C (2Π) $\frac{3}{2}$ (42800) ^a B (2Σ) $\frac{1}{2}$ 40840 ^d A (2Π) X (2Σ) 0		($\mu = 15.4910711$) (608) ^a Rydberg state arising ^b from Kr($3P$) + F($2P$). (356) ^a Ionic state arising ^b from Kr $^+$ ($2P_{1/2}$) + F $^-$. (349) ^a } Ionic states arising ^b from Kr $^+$ ($2P_{3/2}$) + F $^-$. ^e 310 ^d } Repulsive state (11). Repulsive state with rather flat potential function (3)(10)(11).				(1.83) ^a (2.47) ^a (2.44) ^a (2.27) ^f		D \rightarrow X, ^c B \rightarrow X, ^g ESR spectrum ^h	45340 40230	APR 1977 (8)(12) (4)(5)(6) (10) (1)
(84)Kr $19F^+$ X $1\Sigma^+$		$D_0^0 \geq 1.58$ eV ⁱ (621) ^j (8.3) ^j (0.355) ^j (0.0044) ^j (1.752) ^j								APR 1977

KRb: ^aInterpolated values based on the constants for K₂ and Rb₂ (2).

- (1) Walter, Barratt, PRS A 119, 257 (1928).
- (2) Cavaliere, Ferrante, Lo Cascio, JCP 62, 4753 (1975).

KrBr, KrCl:

^aIn emission from low-pressure (0.5-5 torr) reactions of metastable Kr atoms with Br₂ or CH₂Br₂, Cl₂ or CCl₄ (1). The KrCl bands were also observed in electron-beam-excited mixtures of Ar and Kr+Cl₂ (2). The upper states are ionic states arising from Kr⁺+Br⁻ or Cl⁻ although the adiabatic dissociation products are Kr(³P₂) + Br or Cl; the dissociation energies can be estimated as 3.93 eV for KrBr and 4.33 eV for KrCl and are very similar to those of the ground states of RbBr and RbCl.

- (1) Golde, JMS 58, 261 (1975).
- (2) Murray, Powell, APL 29, 252 (1976).

KrF, KrF⁺:

^aTheoretical calculations of (11). T_e relative to the Kr(¹S)+F(²P_{3/2}) limit. For the D state a vibrational frequency of ~336 was observed in argon matrices (9).

^bIn the diabatic sense.

^cIn reactions of metastable Kr atoms with small fluorine containing molecules (8) and from electron-beam-excited mixtures of Ar and Kr+NF₃ (12). Also in absorption of matrix isolated KrF (7)(9).

^dFrom the analysis through trial-and-error theoretical simulations of the structured continuum observed at moderate to high pressures (10). An earlier interpretation (5) of the much broader peaks observed at low pressure

KrF, KrF⁺ (continued):

lead to $w_e \approx 280 \text{ cm}^{-1}$. The theoretical calculations of (11) give 341 cm^{-1} . In neon and argon matrices $w_e \approx 340$ and 315 , respectively (9).

^eThe B state dissociates adiabatically to Kr(³P₂)+F; D₀' $\approx 4.85 \text{ eV}$ is very similar to the ground state dissociation energy of RbF.

^fEstimated value used by (10) in the analysis of the structured continuum. The theoretical value (11) is 2.51 \AA .

^gIn emission from electron-beam-excited mixtures of Ar and Kr+F₂ at moderate to high pressures. The low-pressure spectrum observed in reactions of metastable Kr atoms with F₂ or N₂F₄ (5) may also contain contributions from C→X. Also observed in matrix absorption (7)(9).

^hObserved in γ -irradiated KrF₄ at low temperature (77 K) confirming that the ground state is ²Σ. KrF seems to be stabilized in the solid.

ⁱFrom mass-spectrometric studies (2); ab initio calculations (3) yield D₀⁰ = 1.90 eV.

^jTheoretical values (3); no spectroscopic data available.

- (1) Falconer, Morton, Streng, JCP 41, 902 (1964).
- (2) Berkowitz, Chupka, CPL 7, 447 (1970).
- (3) Liu, Schaefer, JCP 55, 2369 (1971).
- (4) Brau, Ewing, JCP 63, 4640 (1975).
- (5) Golde, JMS 58, 261 (1975).
- (6) Tisone, Hays, Hoffman, OC 15, 188 (1975).
- (7) Ault, Andrews, JCP 64, 3075 (1976).
- (8) Velazco, Kolts, Setser, JCP 65, 3468 (1976).
- (9) Ault, Andrews, JCP 65, 4192 (1976).
- (10) Tellinghuisen, Hays, Hoffman, Tisone, JCP 65, 4473 (1976).
- (11) Dunning, Hay, APL 28, 649 (1976).
- (12) Murray, Powell, APL 29, 252 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(84)Kr ¹ H ⁺ X $1\Sigma^+$										APR 1977 A <

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(39) $K(^{132})\text{Xe}$		$(\mu = 30.0786526) \quad D_e^0 = 0.013_8 \text{ eV}^a$						C \rightarrow X,	JAN 1977 (3)	
C 2Σ	}	Continuous emission with maximum at 19207 cm^{-1} , shifted by 1820 cm^{-1} from the forbidden K $5s - 4s$ line at 21027 cm^{-1} .								
B 2Σ		Interatomic potential calculations (2).								
A 2Π										
X $2\Sigma^+$										
							5.2^a			

KrH⁺: ^aFrom a study of the proton transfer reaction $H_3^+ + Kr = KrH^+ + H_2$, and based on $D_0(H_2 - H^+)$ (3). From elastic scattering of protons by Kr (1) and (2) have derived $D_e = 4.60$ and 4.45 eV, resp..

^bAverage value obtained from proton scattering (1)(2).

- (1) Rich, Bobbio, Champion, Doverspike, PR A 4, 2253 (1971).
- (2) Weise, Mittman, Ding, Henglein, ZN 26 a, 1122 (1971).
- (3) Payzant, Schiff, Bohme, JCP 63, 149 (1975).

KrO: (1) Cooper, Cobb, Tolnas, JMS 2, 223 (1961).
(2) Kugler, AP(Leipzig) (7) 14, 137 (1964).

KrXe, KrXe⁺:

^aFrom the "excess properties" of Kr-Xe mixtures (3).

^bTheoretical values (6), calculated from the potential of (3).

- (1) Friedl, ZN 14 a, 848 (1959); 15 a, 398 (1960).
- (2) See ref. (2) of KrO.
- (3) Lee, Henderson, Barker, MP 29, 429 (1975).
- (4) Tanaka, Yoshino, Freeman, JCP 62, 4484 (1975).
- (5) Verkhovtseva, Ovechkin, Fogel, CPL 30, 120 (1975).
- (6) Bobetic, Barker, JCP 64, 2367 (1976).

KXe: ^aFrom atomic scattering data (1).

- (1) Buck, Pauly, ZP 208, 390 (1968).
- (2) Baylis, JCP 51, 2665 (1969).
- (3) Tam, Moe, Bulos, Happer, OC 16, 376 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{139}\text{La}^1\text{H}$										
		$\mu = 1.00056569$								SEP 1976
b 3ϕ	$\begin{smallmatrix} 4 \\ 3 \\ 2 \end{smallmatrix}$			$\begin{bmatrix} 3.8939 \\ 3.8774 \end{bmatrix}^a$	$\begin{matrix} 0.0892 \\ 0.1071 \end{matrix}$	$\begin{bmatrix} 1.28 \\ 1.40 \end{bmatrix}$	$\begin{bmatrix} 2.0801 \\ 2.0845 \end{bmatrix}$	b \leftrightarrow a,	$\begin{matrix} 16346.74 \text{ Z} \\ 16006.73 \text{ Z} \end{matrix}$	(1)*
a 3Δ	$\begin{smallmatrix} 3 \\ 2 \\ 1 \end{smallmatrix}$			$\begin{bmatrix} 3.8477 \\ 3.8431 \end{bmatrix}$	$\begin{matrix} 0.0764 \\ 0.0773 \end{matrix}$	$\begin{bmatrix} 1.18 \\ 1.20 \end{bmatrix}$	$\begin{bmatrix} 2.0925 \\ 2.0938 \end{bmatrix}$			
C 1Σ				$[3.8162]^a$		$[0.50]$	$[2.1012]$	C \rightarrow A,	18595.10 Z	(1)*
B 1Δ				$[3.8232]^a$		$[2.0]$	$[2.0992]$	B \leftrightarrow A,	15618.76 Z	(1)*
A 1Π				$[3.7837]^b$		$[1.12]$	$[2.1102]$			
$^{139}\text{La}^2\text{H}$										
		$\mu = 1.98531572$								SEP 1976
b 3ϕ	$\begin{smallmatrix} 4 \\ 3 \\ 2 \end{smallmatrix}$			$\begin{bmatrix} 1.9743 \\ 1.9691 \end{bmatrix}^a$	$\begin{matrix} 0.0331 \\ 0.0403 \end{matrix}$	$\begin{bmatrix} 0.35 \\ 0.42 \end{bmatrix}$	$\begin{bmatrix} 2.0738 \\ 2.0766 \end{bmatrix}$	b \rightarrow a,	$\begin{matrix} 16359.92 \text{ Z} \\ 16010.97 \text{ Z} \end{matrix}$	(1)*
a 3Δ	$\begin{smallmatrix} 3 \\ 2 \\ 1 \end{smallmatrix}$			$\begin{bmatrix} 1.9523 \\ 1.9510 \end{bmatrix}$	$\begin{matrix} 0.0274 \\ 0.0282 \end{matrix}$	$\begin{bmatrix} 0.31 \\ 0.34 \end{bmatrix}$	$\begin{bmatrix} 2.0855 \\ 2.0862 \end{bmatrix}$			
B 1Δ				$[1.9261]^a$		$[0.57]$	$[2.0996]$	B \rightarrow A,	15611.92 Z	(1)*
A 1Π				$[1.9346]^c$		$[0.35]$	$[2.0950]$			

La₂: ^aThermochemical value (mass-spectrom.)(1).
 (1) Verhaegen, Smoes, Drowart, JCP 40, 239 (1964).
 (2) Carrette, Blondeau, CR B 269, 16 (1969).

La¹H, La²H:

^aEmission breaks off at relatively low J' values.

^b Λ -type doubling, $\Delta v = 0.0023 J(J+1)$.

^c Λ -type doubling, $\Delta v = 0.00115 J(J+1)$.

(1) Bernard, Bacis, CJP 54, 1509 (1976).

LaF: ^aNot certain whether X 1Σ or a 3Δ is the ground state.

^bStrong interaction between the two 1Σ states.

^c Λ -type doubling.

(1) Shenyavskaya, Gurvich, Mal'tsev, VMUK 20(4), 10 (1965).

(2) Barrow, Bastin, Moore, Pott, Nature 215, 1072 (1967).

(3) Shenyavskaya, Gurvich, Mal'tsev, OS(Engl. Transl.) 24, 556 (1968).

(4) Barrow, Lee, Partridge, unpubl. } quoted by Barrow in

(5) Hauge, unpubl. } DONNSPEC (1970).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	v ₀₀	
¹³⁹ La ¹⁶ O		μ = 14.3433002		D ₀ ⁰ = 8.23 eV ^a		I.P. = 4.9 ₅ eV ^b				FEB 1975 A
F (2Σ)	28015	858	H 3.7	c				F→X, V	28035 H	(6)* (7)(20)
D (2Σ)	(27749)	(790) ^d	H 3	c				D→X, V	(27735) ^d H	(6)* (7)(20)
C 2Π _r	22849.0 e	798.4 ^f	Z 2.2 ₀ ^h	0.3520 ⁱ	0.0017	[2.8] ^j	1.829 ₅	C→A', ^k V	14671.19 ^l Z	(6)*(7)(25)*
	22631.2	792.5 ^g	(2.2 ₁) ^h	0.3503 ⁱ	0.0016				15150.00 ^l Z	(27)(32)
B 2Σ ⁺	17879.1	[730.4]	Z 2.04 ^m	0.3413 ⁿ	0.0017	[2.5]	1.855 ₇	B↔X, R	17837.8 Z	(1)(2)(3)* (4)* (6)* (7)(9)(10)* (11)(13)(19) (21)(28)(30) (32) (22)[La ¹⁸ O]
A 2Π _r	13525.6 o	[757.17]	Z 2.0 ₁ ^p	[0.3463] ^q	r	[3.1]	[1.842 ₂]	A↔X, R	13497.63 ^l Z	(1)(2)* (6)*
	12663.3	761.8 ^p	2.1 ₂						12635.65 ^l Z	(7)(10)* (11)(19)(32)
A' 2Δ _r	8191.2	771.6 ^f	Z 2.3 ₀ ^h	0.3444	0.0017	[2.8] ^t	1.848 ₅			
	7493.4	768.0 ^s	(2.1 ₇) ^h	0.3435	0.0016					
X 2Σ ⁺ u	0	[812.7 ₅]	Z 2.22 ^{mh}	0.3526 ^v	0.0014	2.6	1.825 ₇	ESR sp. ^w		

LaO: ^aThermochemical value (mass-spectrom.)(5)(8)(15)(16)(17)(18)(29); photoionization [Parr and Inghram, quoted in (23)].

^bElectron impact appearance potential (31).

^cTentative rotational analysis (24).

LaO (continued):

^d(20) favour a slightly different vibrational analysis, increasing v' by 1 and choosing $v_{00} = 26949$.

^e $A_0 = +221.44$.

LaO (continued):

- ^fFrom band origins (25) as well as band heads (7) in C-A', the latter corrected for head-origin separations.
- ^gFrom band heads in the 0-0 sequence of C-X (6) after correcting for head-origin separations.
- ^hSlightly different constants in (27).
- ⁱLarge Λ -type doubling in $^2\Pi_{1/2}$: $\Delta v_{ef}(v=0) = +0.121(J+\frac{1}{2}) - \dots$; in $^2\Pi_{3/2}$: $\Delta v_{ef}(v=0) = +0.80 \times 10^{-6}(J-\frac{1}{2})(J+\frac{1}{2})(J+3/2)$.
- ^j $D_1 = 2.5 \times 10^{-7}$.
- ^kSystems $G \rightarrow ?$ and $E \rightarrow ?$ of (7).
- ^l $J'=0$ relative to $N''=0$ or $J''=0$.
- ^mFrom band heads and calculated head-origin separations in B-X.
- ⁿLarge spin doubling in B $^2\Sigma^+$: $\Delta v_{12} = (-)0.256(N+\frac{1}{2})$; small hyperfine structure [see (28)].
- ^o $A_0 = +862.6$.
- ^pFrom band heads and calculated head-origin separations in A-X.
- ^qLarge Λ -type doubling in $^2\Pi_{1/2}$: $\Delta v_{ef} = +0.267(J+\frac{1}{2})$.
- ^r $B_1(^2\Pi_{3/2}) = 0.3449$.
- ^sFrom Q as well as P heads, the latter corrected for head-origin separations, in the 0-0 sequence of C $^2\Pi_{1/2} - A'$ $^2\Delta_{3/2}$.
- ^t $D_1 = 2.5 \times 10^{-7}$.
- ^uMatrix studies at 4 K (14)(19) confirm that X $^2\Sigma^+$ is the ground state. See also (12)(13).
- ^vSmall spin doubling in X $^2\Sigma^+$: $\Delta v_{12} = +0.00257(N+\frac{1}{2})$ (28); large hyperfine structure, $4b = 0.494$ (10)(26)(28).
- ^wIn Ar matrix at 4 K (14)(19).
- (1) Jevons, PPS 41, 520 (1929).
 - (2) Meggers, Wheeler, JRNBS 6, 239 (1931); 2, 268 (1932).
 - (3) Piccardi, GCI 63, 127 (1933).
 - (4) Gatterer, RS 1, 153 (1942).
 - (5) Chupka, Inghram, Porter, JCP 24, 792 (1956).

LaO (continued):

- (6) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (7) Hautecler, Rosen, BCSARB 45, 790 (1959).
- (8) Goldstein, Walsh, White, JPC 65, 1400 (1961).
- (9) Tawde, Chandratreya, CS 30, 137 (1961).
- (10) Åkerlind, AF 22, 65 (1962).
- (11) Ortenberg, Glasko, Dimitriev, SAAJ 8, 258 (1964).
- (12) Berg, Wharton, Klemperer, Büchler, Stauffer, JCP 43, 2416 (1965).
- (13) Brewer, Walsh, JCP 42, 4055 (1965).
- (14) Kasai, Weltner, JCP 43, 2553 (1965).
- (15) Smoes, Drowart, Verhaegen, JCP 43, 732 (1965).
- (16) Ames, Walsh, White, JPC 71, 2707 (1967).
- (17) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).
- (18) Drowart, Pattoret, Smoes, PBCS, No. 8, 67 (1967).
- (19) Weltner, McLeod, Kasai, JCP 46, 3172 (1967).
- (20) Carette, Houdart, CR B 271, 110 (1970).
- (21) Murthy, Murthy, JP B 3, L15 (1970); 5, 714 (1972).
- (22) Suárez, JP B 3, 729 (1970); CPL 16, 515 (1972).
- (23) Uy, Drowart, HTS 2, 293 (1970).
- (24) Carette, Houdart, CR B 272, 595 (1971).
- (25) Green, JMS 38, 155 (1971).
- (26) Green, CJP 42, 2552 (1971).
- (27) Green, JMS 40, 501 (1971).
- (28) Bacis, Collomb, Bessis, PR A 8, 2255 (1973).
- (29) Ackermann, Rauh, JCP 60, 2266 (1974).
- (30) Marañón, Suárez, SpL 7, 303 (1974).
- (31) Rauh, Ackermann, JCP 60, 1396 (1974).
- (32) Schoonveld, Sundaram, ApJ(Suppl.) 27(246), 307 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{139}\text{La}^{103}\text{Rh}$		$\mu = 59.113028$		$D_0^0 = 5.4_4 \text{ eV}^a$						FEB 1975
$^{139}\text{La}^{32}\text{S}$		$\mu = 25.9899651$		$D_0^0 = 5.9_1 \text{ eV}^a$						FEB 1975
B $^2\Sigma^+$	13790.17	410.07 ₅	H 0.94	[0.11099] ^b	(0.00034)	[0.031]	[2.4174]	B \leftrightarrow X, R	13766.86 Z	(5)
X $^2\Sigma^+$	0	456.7 ₀	H 0.96 ₅	[0.11693] ^c	(0.00034)	[0.030]	[2.3552]			(5)
$^{139}\text{La}^{(80)}\text{Se}$		($\mu = 50.730136_7$)		$D_0^0 = 4.9_3 \text{ eV}^a$						FEB 1975
$^{139}\text{La}^{(130)}\text{Te}$		($\mu = 67.127825$)		$D_0^0 = 3.9_1 \text{ eV}^a$						FEB 1975
$^{139}\text{La}^{89}\text{Y}$		$\mu = 54.209522$		$D_0^0 = 2.0_4 \text{ eV}^a$						FEB 1975
$^7\text{Li}_2$		$\mu = 3.5080024$		$D_0^0 = 1.04_6 \text{ eV}^a$		I.P. = 5.0 ₀ eV ^b				MAR 1977 A
				Fragments of other absorption band systems in the ultraviolet.						(5)
D $^1\Pi_u$	(34518) ^c	[201.68] ^c Z		0.4628 ^d	0.0073	11.4	3.222	D \leftarrow X, R	34443.58 ^c Z	(11)(17)
C $^1\Pi_u$	30550.6	237.9 Z	3.35 ^e	0.5075 ⁱ	0.0097 ₃ ^f	9	3.077	C \leftarrow X, R	30493.6 Z	(5)(9)(11) (12)(16)
B $^1\Pi_u$	20436.01	270.12 Z	2.67 ₃ ^g	0.5577 ^{hi}	0.0085 ^j	9.45 ^k	2.935	B \leftrightarrow X, ^l R	20395.32 Z	(1)* (3)(4) (18)(19)(20) (21)
A $^1\Sigma_u^+$	14068.35	255.47 Z	1.58 ₂ ^m	0.4975 ₀ ⁱ	0.0054 ₀	7.54 ⁿ	3.107 ₉	A \leftarrow X, ^l R	14020.63 Z	(6)(8)*
a $^3\Sigma_u^+$		Not observed; predicted potential minimum of $\sim 300 \text{ cm}^{-1}$ at 4.3 \AA (22).								
X $^1\Sigma_g^+$	0	351.43 Z	2.610 ^o	0.67264 ⁱ	0.00704 ^p	9.87 ^q	2.6729	Mol. beam magn. reson. ^r		(10)(13)

LaRh: ^aThermochemical value (mass-spectrom.)(1).

(1) Cocke, Gingerich, Kordis, HTS 5, 474 (1973).

LaS: ^aThermochemical value (mass-spectrom.)(1)(2)(3)(4).

^bLarge spin-splittings, $\gamma_0 = (-)0.0962_7$.

^cLarge hyperfine splittings, $4b = 0.47 \text{ cm}^{-1}$.

(1) Cater, Lee, Johnson, Rauh, Eick, JPC 69, 2684 (1965).

(2) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).

(3) Cater, Steiger, JPC 72, 2231 (1968).

(4) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

(5) Marciano, Barrow, JP B 3, L121 (1970).

LaSe: ^aThermochemical value (mass-spectrom.)(1)(2).

(1) See ref. (4) of LaS.

(2) Ni, Wahlbeck, HTS 4, 326 (1972).

LaTe: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (4) of LaS.

LaY: ^aThermochemical value (mass-spectrom.)(1).

(1) Verhaegen, Smoes, Drowart, JCP 40, 239 (1964).

Li_2 , Li_2^+ , Li_2^- :

^aValue recommended by (33). Extrapolation of the ground state vibrational levels, taking into account the contribution due to long-range forces, gives 8473 cm^{-1} [1.051 eV , see (33)]. The latest thermochemical value [mass-spectrom.(32)] is 1.11 eV ; see also (2) who obtained 1.03 eV using a molecular beam method.

^bAverage of a photoionization (15) and electron impact (32) appearance potential (5.15 and 4.86 eV , resp.). The Rydberg series B,C,D... extrapolates to 4.99 eV (26).

Li_2 , Li_2^+ , Li_2^- (continued):

^cVibrational numbering uncertain.

^dRotational constants from Q branches only; see also ^c.

^e $\omega_e y_e = + 0.064$.

^f $\gamma_e = + 0.00015_4$. Rotational constants from Q branches only; (12) gives $B(R,P) - B(Q) = + 0.0024$.

^g $\omega_e y_e = - 0.082_5$. Vibrational constants recalculated from band origins ($v'=0...4$) of (20). Slightly different constants in (3) from a low-resolution magnetic rotation spectrum including much higher vibrational levels. The $B^1\Pi_u$ state has a potential maximum of $\sim 0.09 \text{ eV}$ (7)(18)(29); the theoretical calculations of (35) predict a barrier of 0.0724 eV at 5.61 \AA .

^hSlightly different constants in (25); Λ -type doubling

$\Delta v_{ef} \approx + 0.00016 J(J+1)$.

ⁱRKR potential curves (14).

^j $\gamma_e \approx - 0.00014$.

^k $\beta_e = + 0.14 \times 10^{-6}$.

^lThe B-X and A-X systems of $^6\text{Li}_2$ have been analysed by (24) and (23), respectively.

^m $\omega_e y_e = + 0.0025$.

ⁿ $H_e = + 1.23 \times 10^{-10}$.

^o $\omega_e y_e = + 0.00295$, $\omega_e z_e = - 0.000636$; from the B-X fluorescence spectrum (18), including levels from $v=0$ to 18.

^p $\gamma_e = - 0.00004$ ($v=0...4$) (8). For $v > 10$ B_v and D_v are better represented by $B_v = B_{10} - 0.0077(v-10) - 0.00016(v-10)^2$ and

$D_v = D_{10} + 0.22 \times 10^{-6}(v-10)$ (18).

^q $H_e = + 1.54 \times 10^{-10}$. See also P.

^r $g_J = 0.1079_7 \mu_N$ (13). Li nuclear electric quadrupole coupling constant (10).

(continued on p. 376)

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State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
${}^7\text{Li}_2^+$										MAR 1977
${}^7\text{Li}_2^-$										MAR 1977
$({}^7)\text{Li}^{40}\text{Ar}$										JAN 1977
B ${}^2\Sigma$ A ${}^2\Pi$ (14150) X ${}^2\Sigma^+$ 0										(5)
$({}^7)\text{Li}^{40}\text{Ar}^+$										JAN 1977
${}^7\text{Li}^{79}\text{Br}$										JAN 1977
A X ${}^1\Sigma^+$ 0										(5)
										(4)(7)
										(3)(10)(12)
										(12)(16)(17)
										(13)

Li_2 , Li_2^+ , Li_2^- (continued): $s_{D_0^0}(\text{Li}_2) + \text{I.P.}(\text{Li}) - \text{I.P.}(\text{Li}_2)$.

^tFrom $D_0^0(\text{Li}_2)$ and the electron affinities of Li_2 and Li .

^uTheoretical electron affinity of Li_2 from an ab initio calculation by (34).

A value of 0.90 eV was computed earlier by (28), but see (34).

Li_2 , Li_2^+ , Li_2^- (continued):

- (1) Harvey, Jenkins, PR 35, 789 (1930).
- (2) Lewis, ZP 62, 786 (1931).
- (3) Loomis, Nusbaum, PR 38, 1447 (1931).
- (4) McKellar, PR 44, 155 (1933).
- (5) Vance, Huffman, PR 47, 215 (1935).
- (6) Almy, Irwin, PR 49, 72 (1936).
- (7) King, Van Vleck, PR 55, 1165 (1939).
- (8) McKellar, Jenkins, PDAO 7, 155 (1939).
- (9) Sinha, PPS 60, 443 (1948).
- (10) Logan, Cote, Kusch, PR 86, 280 (1952).
- (11) Barrow, Travis, Wright, Nature 187, 141 (1960).
- (12) Velasco, ARSEFQ A 56, 175 (1960).
- (13) Brooks, Anderson, Ramsey, PRL 10, 441 (1963);
PR A 136, 62 (1964).
- (14) Krupenie, Mason, Vanderslice, JCP 39, 2399 (1963).
- (15) Foster, Leckenby, Robbins, JP B 2, 478 (1969).
- (16) Rico, OPA 2 (1), 33 (1969).
- (17) Mercier, Rico, Velasco, OPA 2 (2), 96 (1969).
- (18) Velasco, Ottinger, Zare, JCP 51, 5522 (1969).
- (19) Ottinger, Velasco, Zare, JCP 52, 1636 (1970).
- (20) Velasco, Ruano, Rico, OPA 3 (3), 159 (1970).
- (21) Ottinger, Poppe, CPL 8, 513 (1971).
- (22) Kutzelnigg, Staemmler, Gélus, CPL 13, 496 (1972).
- (23) Velasco, Rivero, OPA 5 (2), 76 (1972).
- (24) Velasco, Morales, Publ. Inst. Optica "Daza de
Valdes" Madrid, No. 36 (1972); OPA 6 (1), 52 (1973).
- (25) Velasco, Ennen, Ottinger, OPA 6 (2), 11 (1973).
- (26) Velasco, OPA 6 (2), 16 (1973).
- (27) Bottcher, Dalgarno, CPL 36, 137 (1975).
- (28) Andersen, Simons, JCP 64, 4548 (1976).
- (29) Olson, Konowalow, CPL 39, 281 (1976).
- (30) Müller, Jungen, CPL 40, 199 (1976).

Li_2 , Li_2^+ , Li_2^- (continued):

- (31) Kirby-Docken, Cerjan, Dalgarno, CPL 40, 205 (1976).
- (32) Wu, JCP 65, 2040, 3181 (1976).
- (33) Stwalley, JCP 65, 2038 (1976).
- (34) Dixon, Gole, Jordan, JCP 66, 567 (1977).
- (35) Kahn, Dunning, Winter, Goddard, JCP 66, 1135 (1977).

LiAr , LiAr^+ :

- ^aFrom differential (3) and total (2) scattering cross sec-
^bSee the semiempirical calculations of (1). | tions.
^cMorse potential parameters (average of two suggested values)
from the analysis of the far-wing fluorescence spectrum
longward of the Li resonance line at 14904 cm^{-1} (5). See
^dSee the potential energy curves in (2)(3)(5). | also (6).
^eFrom Li^+ -off-Ar differential scattering measurements (4).

- (1) Baylis, JCP 51, 2665 (1969).
- (2) Ury, Wharton, JCP 56, 5832 (1972).
- (3) Klingbeil, JCP 59, 797 (1973).
- (4) Böttner, Dimpfl, Ross, Toennies, CPL 32, 197 (1975).
- (5) Scheeps, Ottinger, York, Gallagher, JCP 63, 2581 (1975).
- (6) Scheeps, Gallagher, JCP 65, 859 (1976).

LiBr : ^aThermochemical value (8)(9).

- ^bMaximum of a very broad photoelectron peak with two addi-
tional ill-defined peaks at 10.6 and 11.6 eV, the latter
possibly due to the dimer $(\text{LiBr})_2$ (19).
^cAbsorption cross sections (14).
^d $\omega_e y_e = +0.02$; vibrational constants from the infrared
spectrum of the natural isotopic mixture.
^e $\gamma_e = +0.0000244$; rotational constants evaluated (12) from
the microwave results for $^6\text{Li}^{79}\text{Br}$.
^fFor IR spectrum in inert gas matrices see (11).
(continued on p. 379)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$7\text{Li}^{35}\text{Cl}$										
		$\mu = 5.8435744$		$D_0^0 = 4.8_4 \text{ eV}^a$						JAN 1977
K $3p\pi$ $^2\Pi$	513500	1090	} First members of two Rydberg series converging to the Li $1s$ ionization limit of LiCl at $\sim 66 \text{ eV}$ (532300 cm^{-1}); vibrational numbering not established.					K \leftarrow X,	513700	(28)
J 3σ $^2\Sigma$	505900	1030						J \leftarrow X,	506100	(28)
I $2p\pi$ $^2\Pi$	479200	850						I \leftarrow X,	479300	(28)
H 2σ $^2\Sigma$	463900	950						H \leftarrow X,	464000	(28)
		The energy loss spectrum of 25 keV electrons has peaks at 5.3, 7.2, and 8.9 eV. Continuous absorption above 40000 cm^{-1} , first maximum ^b at 42800 cm^{-1} . ^c Diffuse absorption bands at 35642, 35032, 34482 cm^{-1} .								(19)
A										(1)(18)
X $1\Sigma^+$	0	643.31^d	4.50_1^d	0.7065222_4	0.0080096_1^e	3.4087^f	2.020673^g	A \leftarrow X		(6)
		Rot.-vibr. sp. ^h								(5)(9)
		Rotation sp.								(14)(21)
		Mol. beam rf electric ⁱ and magn. reson. ^j								(4)(20)(22)(24)(17)
$(7)\text{Li}(^{35})\text{Cl}^-$										
				$D_0^0 = 1.8_4 \text{ eV}^k$		I.P. = 0.61 eV^l				JAN 1977
X $2\Sigma^+$	0	$(480)^l$					2.18^m			

LiCl , LiCl^- :

^aThermochemical value (10)(11)(15). A slightly higher value was suggested by (7).

^bAlso observed in the electron energy loss spectrum.

^cAbsorption cross sections (18).

^dCalculated (21) from the rotational constants by use of Dunham's theory. From the infrared spectrum of the isotopic mixture (9) obtain $w_e = 641.1$, $w_e x_e = 4.2$. For $^6\text{Li}^{35}\text{Cl}$ (12) find $w_e \approx 705$ by the molecular beam electric reson. method.

^e $r_e = +0.00003966$.

^f $\beta_e = -0.0190 \times 10^{-6}$.

^gFrom the effective B_e . Using the data of (21) for the four LiCl isotopes (23) has determined r_e at the minimum of the Born-Oppenheimer potential as 2.020700 \AA .

^hIR spectrum of matrix isolated LiCl (13)(16).

ⁱElectric dipole moment of $^6\text{Li}^{35}\text{Cl}$: $\mu_{eL}[D] = 7.085_3 + 0.0868(v+\frac{1}{2}) + 0.0005_6(v+\frac{1}{2})^2$ (20), see also (4)(14). For electric quadrupole and other hyperfine coupling constants see (4)(22). The Zeeman spectrum was also studied by the

LiCl, LiCl⁻ (continued):

molecular beam electric reson. method (24); $g_J(^7\text{Li}^{35}\text{Cl}) = +0.10042$ and $+0.10064 \mu_N$ for $v=0$ and 1 , resp., superseding an earlier value by the magnetic resonance method (17).

^jNuclear reorientation spectrum of Li (2)(3)(8).

^kFrom $D_0^0(\text{LiCl})$ and the electron affinities of LiCl and Cl.

^lFrom the photoelectron spectrum of LiCl⁻ (25); I.P. is reasonably close to the calculated electron affinity of LiCl [0.54 eV (26)]; see also (27).

^mThe relative intensities of the photoelectron peaks have been compared (25) with calculated Franck-Condon factors.

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Kusch, PR 75, 887 (1949).
- (3) Logan, Côté, Kusch, PR 86, 280 (1952).
- (4) Marple, Trischka, PR 103, 597 (1956).
- (5) Klemperer, Rice, JCP 26, 618 (1957).
- (6) Berry, Klemperer, JCP 26, 724 (1957).
- (7) Gurvich, Veits, BASPS 22, 670 (1958).
- (8) Kusch, JCP 30, 52 (1959).
- (9) Klemperer, Norris, Büchler, Emslie, JCP 33, 1534 (1960).

- (10) Brewer, Brackett, CRev 61, 425 (1961).
- (11) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (12) Moran, Trischka, JCP 34, 923 (1961).
- (13) Snelson, Pitzer, JPC 67, 882 (1963).
- (14) Lide, Cahill, Gold, JCP 40, 156 (1964).
- (15) Hildenbrand, Hall, Ju, Potter, JCP 40, 2882 (1964).
- (16) Schlick, Schnepp, JCP 41, 463 (1964).
- (17) Mehran, Brooks, Ramsey, PR 141, 93 (1966).
- (18) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (19) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (20) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
- (21) Pearson, Gordy, PR 177, 52 (1969).
- (22) Gallagher, Hilborn, Ramsey, JCP 56, 5972 (1972).
- (23) Watson, JMS 45, 99 (1973).
- (24) Freeman, Johnson, Ramsey, JCP 61, 3471 (1974).
- (25) Carlsten, Peterson, Lineberger, CPL 37, 5 (1976).
- (26) Jordan, Luken, JCP 64, 2760 (1976).
- (27) Jordan, JCP 65, 1214 (1976).
- (28) Radler, Sonntag, Chang, Schwarz, CP 13, 363 (1976).

LiBr (continued):

^gDipole moment of $^6\text{Li}^{79}\text{Br}$: $\mu_{el}[D] = 7.226_2 + 0.083_2(v+\frac{1}{2}) + 0.0005_7(v+\frac{1}{2})^2$ (12). For electric quadrupole and other hyperfine coupling constants of the various isotopes see (12)(16) (17). The Zeeman spectrum was studied by the electric resonance method (18); $g_J(^7\text{Li}^{79}\text{Br}) = 0.11206$ superseding an earlier value by the magnetic resonance method (13); also $^{79,81}\text{Br}$ nuclear magnetic moments.

^hLi nuclear reorientation spectrum (1)(2)(6).

(1)(2) See ref. (2)(3), resp., of LiCl.

- (3) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (4)...(9) See ref. (5)(6)(8)...(11), resp., of LiCl.
- (10) Rusk, Gordy, PR 127, 817 (1962).
- (11) See ref. (16) of LiCl.
- (12) Hebert, Breivogel, Street, JCP 41, 2368 (1964).
- (13)...(15) See ref. (17)...(19), resp., of LiCl.
- (16) Hebert, Street, PR 178, 205 (1969).
- (17) Hilborn, Gallagher, Ramsey, JCP 56, 855 (1972).
- (18) Cecchi, Ramsey, JCP 60, 53 (1974).
- (19) Goodman, Allen, Cusachs, Schweitzer, JESRP 3, 289 (1974).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(7) Li^{133}Cs		$(\mu = 6.6642051) \quad D_e^0 = (0.72) \text{ eV}^a$								JAN 1977
B	(16477)	(77)	H	Fragment				B \leftarrow X,	16432	H (1)(2)
X	$1\Sigma^+$ 0	(167)	H				(3.54) ^b			
$^7\text{Li}^{19}\text{F}$		$\mu = 5.1238103 \quad D_0^0 = 5.91 \text{ eV}^a$								JAN 1977
K	$3p\pi \quad 2\Pi \quad 510700$	1420	} First members of two Rydberg series converging to the Li 1s ionization limit of LiF at 65.5 eV (528300 cm^{-1}); vibrational numbering not established.					K \leftarrow X,	510900	(31)
J	$3\sigma \quad 2\Sigma \quad 502200$	1400						J \leftarrow X,	502500	(31)
I	$2p\pi \quad 2\Pi \quad 477500$	1240						I \leftarrow X,	477600	(31)
H	$2\sigma \quad 2\Sigma \quad 458600$	(1000)						H \leftarrow X,	458600	(31)
		Peaks in the electron energy loss spectrum at 6.6, 8.7, 10.9, 62.0 eV.								(22)
		<u>Ab initio</u> studies of the lowest 1Σ states (including the ground state), curve crossings (28)(29)(32).								
X	$1\Sigma^+$ 0	910.34 ^b	Z	7.929 ^b	1.3452576	0.0202868 ^c	1.1754 ^d	1.563864	Rotation-vibr. sp. ^e Rotation sp. Mol. beam rf electric ^f and magn. reson. ^g	(8)(9)(14) (16)(19)(24) (25) (16)(23)(26) (30) (20)

LiCs: ^aFrom Li - Cs total scattering cross sections (3), dependent on the assumed value for r_e .

^bTheoretical value, quoted in (3).

(1) Walter, Barratt, PRS A 110, 257 (1928).

(2) Weizel, Kulp, AP(Leipzig) 4, 971 (1930).

(3) Kanen, Pauly, Vietzke, ZN 26 a, 689 (1971).

LiF: ^aThermochemical value (5)(10)(11)(17).

^bFrom the infrared spectrum [constants corresponding to the J numbering " $M_{\text{orig}} - 2$ " in table III of (9)]. In good agreement with constants calculated from the microwave results:

$\omega_e = 910.25$, $\omega_e x_e = 8.10$.

^c $+ 0.0001558(v + \frac{1}{2})^2 - 3.5 \times 10^{-7}(v + \frac{1}{2})^3$.

LiF (continued):

$$d\beta_e = -0.0124 \times 10^{-5}.$$

^eFor IR frequencies in inert gas matrices see (12)(15)(18)(21). The lifetime of the lowest vibrationally excited level of ⁶LiF, $\tau(v=1) = 14.3$ ms, was determined by (27) using the molecular beam electric resonance method.

^fDipole moment of ⁷LiF: $\mu_{el}[D] = 6.2839 + 0.08153(v+\frac{1}{2}) + 0.000445(v+\frac{1}{2})^2$, $v=0,1,2$ (30); see also (16)(23)(26). For electric quadrupole and other hyperfine coupling constants see (25)(30). Earlier electric resonance work in (2)(3)(4)(13) and (6) who found $g_J(^7\text{LiF}) = +0.0642 \mu_N$ from the Zeeman splitting of the hyperfine structure; see also ^g.

^g $g_J(^7\text{LiF}) = (+)0.0737 \mu_N$ by the magnetic resonance method (20); see also (6). Li NMR spectrum (1)(7).

- (1) Kusch, PR 75, 887 (1949).
- (2) Swartz, Trischka, PR 88, 1085 (1952).
- (3) Braunstein, Trischka, PR 98, 1092 (1955).
- (4) Kastner, Russell, Trischka, JCP 23, 1730 (1955).
- (5) Pugh, Barrow, TFS 54, 671 (1958).
- (6) Russell, PR 111, 1558 (1958).
- (7) Kusch, JCP 30, 52 (1959).
- (8) Klemperer, Norris, Büchler, Emslie, JCP 33, 1534 (1960).
- (9) Vidale, JPC 64, 314 (1960).

- (10) Brewer, Brackett, CREv 61, 425 (1961).
- (11) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (12) Linevsky, JCP 34, 587 (1961); 38, 658 (1963).
- (13) Moran, Trischka, JCP 34, 923 (1961).
- (14) Vasilevskii, Baikov, OS(Engl. Transl.) 11, 21 (1961).
- (15) Snelson, Pitzer, JPC 67, 882 (1963).
- (16) Wharton, Klemperer, Gold, Strauch, Gallagher, Derr, JCP 38, 1203 (1963).
- (17) Hildenbrand, Hall, Ju, Potter, JCP 40, 2882 (1964).
- (18) Schlick, Schnepp, JCP 41, 463 (1964).
- (19) Veazey, Gordy, PR A 138, 1303 (1965).
- (20) Mehran, Brooks, Ramsey, PR 141, 93 (1966).
- (21) Snelson, JCP 46, 3652 (1967).
- (22) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (23) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
- (24) Pearson, Gordy, PR 177, 52 (1969).
- (25) Cupp, Smith, Contini, Woods, Gallagher, PL A 44, 305 (1973).
- (26) Mariella, Herschbach, Klemperer, JCP 58, 3785 (1973).
- (27) Bedding, Moran, PR A 9, 2324 (1974).
- (28) Kahn, Hay, Shavitt, JCP 61, 3530 (1974).
- (29) Botter, Kooter, Mulder, CPL 33, 532 (1975).
- (30) Hebert, Hollowell, JCP 65, 4327 (1976).
- (31) Radler, Sonntag, Chang, Schwarz, CP 13, 363 (1976).
- (32) Yardley, Balint-Kurti, MP 31, 921 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-3}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^7\text{Li}^1\text{H}$										
$\mu = 0.88123833$ $D_0^0 = 2.42871 \text{ eV}^a$ For <u>ab initio</u> calculations of $X^1\Sigma$, $A^1\Sigma$, $B^1\Pi$, $a^3\Sigma$, $b^3\Pi$ (lowest stable triplet state at $\sim 1700 \text{ cm}^{-1}$ below $B^1\Pi$) see (13). Excitation energies and oscillator strengths for higher-lying states have been computed by (19). The most recent ground state studies are those of (17) and (22), the latter including other low-lying $^1\Sigma^+$ states.										JAN 1977 A
B $^1\Pi$	34912	[130.73]	Z ^b	3.383 ^c	0.986 ^e	[2.6] ^f	2.378	B \leftarrow X, R	34312.26 Z	(3)*
A $^1\Sigma^+$	26516	[280.96] ^g	Z	[2.8536] ^{gd}		[1.187] ^g	2.60 ₅	A \leftrightarrow X, ⁱ R	25943.13 Z	(1)
X $^1\Sigma^+$	0	1405.65	Z 23.20 ^j	7.5131 ^d	0.2132 ^k	0.8617 ^l	1.5957	Rot.-vibr. sp.		(2)(4)(5)
								Mol. beam electric ^m and magn. reson.		(7)(12)(18) (8)
$^7\text{Li}^2\text{H}$										
$\mu = 1.56487081$ $D_0^0 = 2.45090 \text{ eV}^a$ I.P. = 7.7 eV^b										JAN 1977
B $^1\Pi$	34908.8	178.70	Z 29.13 ^c	1.904 ^d	0.425 ^e	0.44 ^f	2.379	B \leftarrow X, R	34466.27 Z	(2)(9)
A $^1\Sigma^+$	26513	[205.6] ^g		[1.6125] ^{hi}		[0.3508] ^h	2.59 ₀	A \leftrightarrow X, R	26082.8 Z	(1)(11)
X $^1\Sigma^+$	0	1054.80 ₃	Z 12.93 ₅ ^j	4.239 ₄ ^k	0.100 ₀ ^l	0.2756 ^m	1.5941	Rotation spectrum		(7)
								Mol. beam electric ⁿ and magn. reson.		(5)(8)(13) (6)

Li^1H : ^aFrom the predissociation in $B^1\Pi$; the evaluation by (14) takes into account the long-range potential of this state.

^b $\Delta G(3/2) = 45.9$.

^cPredissociation by rotation; breaking off above $J'=8,5,2$ in $v'=0,1,2$, respectively; see also (14). Dissociation limit at 34492.5 cm^{-1} above $X^1\Sigma$, $v''=0$, $J''=0$.

^dRKR potential curves (6); (9)[A state]; (14)[B state,

combination with long-range tail and exponential inner wall].

^e $\gamma_e = -0.045$.

^f $D_1 = 4.8 \times 10^{-3}$; $H_0 = -1.7 \times 10^{-5}$, $H_1 = -5.6 \times 10^{-5}$.

^g $\Delta G(v+\frac{1}{2})$, B_v , D_v , H_v have been determined up to $v=14$. The ΔG and B_v curve have maxima for $v=9$ and 3 , resp.; $w_e \approx 235$, $w_e x_e \approx -28$, $w_e y_e \approx -4$; $B_e \approx 2.819$, $\alpha_e \approx -0.078$, $\gamma_e \approx -0.026$, and higher order constants.

Li^1H (continued):

^hRadiative lifetimes $\tau(v', J')$: $\tau(2, 3) = 29.4 \text{ ns}$, $\tau(5, 3) = 30.5 \text{ ns}$, $\tau(7, 12) = 36.9 \text{ ns}$ (20); $\tau(5, 5-15) = 31 \text{ ns}$ (21).

ⁱIntensity distribution in the $v'-0$ bands (11); RKR Franck-Condon factors (10). The A-X system of $^6\text{Li}^1\text{H}$ was analyzed by (15).

^j $\omega_e y_e = + 0.163$.

^k $\gamma_e = + 0.00075$; all rotational constants are from $v=0, 1, 2$ only.

^l $\beta_e = - 0.0160 \times 10^{-3}$, see ^k. $H_v = 11.4 \times 10^{-8} - \dots$

^m $\mu_{el}(v=0, 1, 2) = 5.8820, 5.9905, 6.098 \text{ D}$ (7)(12). Hyperfine structure constants (7)(12)(18). Zeeman spectrum (18), $g_J(v=0, J=1) = -0.6584_2$ in agreement with an earlier less precise value obtained by (8) using the magnetic resonance method. For a combination of both theoretical (13) and experimental results see (16).

- (1) Crawford, Jorgensen, PR 47, 932 (1935); 49, 745
- (2) Klemperer, JCP 23, 2452 (1955) | (1936).
- (3) Velasco, CJP 35, 1204 (1957); OPA 7(1), 14 (1974).
- (4) Norris, Klemperer, JCP 28, 749 (1958).
- (5) James, Norris, Klemperer, JCP 32, 728 (1960).
- (6) Fallon, Vanderslice, Mason, JCP 32, 1453 (1960); 33, 944 (1960) [Erratum].
- (7) Wharton, Gold, Klemperer, JCP 33, 1255 (1960); 37, 2149 (1962).
- (8) Lawrence, Anderson, Ramsey, PR 130, 1865 (1963).
- (9) Singh, Jain, PPS 29, 274, 753 (1963).
- (10) Halmann, Laulicht, JCP 46, 2684 (1967).
- (11) Fernandez-Florez, Velasco, OPA 2(3), 123 (1969).
- (12) Rothstein, JCP 50, 1899 (1969).
- (13) Docken, Hinze, JCP 57, 4928, 4936 (1972).

Li^1H (continued):

- (14) Way, Stwalley, JCP 59, 5298 (1973).
- (15) Velasco, Rivero, OPA 7(1), 45 (1974).
- (16) Docken, Freeman, JCP 61, 4217 (1974).
- (17) Meyer, Rosmus, JCP 63, 2356 (1975).
- (18) Freeman, Jacobson, Johnson, Ramsey, JCP 63, 2597 (1975).
- (19) Stewart, Watson, Dalgarno, JCP 63, 3222 (1975).
- (20) Dagdigian, JCP 64, 2609 (1976).
- (21) Wine, Melton, JCP 64, 2692 (1976).
- (22) Yardley, Balint-Kurti, MP 31, 921 (1976).

- Li^2H : ^aFrom the predissociation in $\text{B}^1\Pi$ (9). A thermochemical value (mass-spectrom.) of 2.49 eV was determined by (12).
- ^bElectron impact appearance potential (12).
- ^c $\omega_e y_e = - 3.51$ ($v=0\dots3$) (9).
- ^dAll four observed levels are predissociated by rotation; breaking off above $J'=12, 9, 6, 2$ in $v'=0, 1, 2, 3$. Dissociation limit at 34671.5 cm^{-1} above $\text{X}^1\Sigma$, $v''=0$, $J''=0$.
- ^e $- 0.005(v+\frac{1}{2})^2 - 0.001(v+\frac{1}{2})^3$, $v=0\dots3$ (9).
- ^f $\beta_e = +0.63 \times 10^{-3}$; $H_0 = - 2.5 \times 10^{-6}$, $H_1 = - 5.3 \times 10^{-6}$, $H_2 = - 16.5 \times 10^{-6}$.
- ^gExtrapolated from the observed $\Delta G(v+\frac{1}{2})$ values for $v=1\dots18$. The ΔG curve has a maximum at $v=13$. $\omega_e \approx 181.9$, $\omega_e x_e \approx - 13.4$, $\omega_e y_e \approx - 1.0_3$, ...
- ^hExtrapolated from observations for $v=1\dots17$; H_v values were also determined. The B_v curve goes through a maximum at $v=4$. $B_e \approx 1.6054$, $\alpha_e \approx - 0.0152$, $\gamma_e \approx - 0.0021_1$, ...
- ⁱRKR potential curves (3)(4).
- ^j $+ 0.0392_3(v+\frac{1}{2})^3 + 0.00325_3(v+\frac{1}{2})^4 - 0.000148_9(v+\frac{1}{2})^5$; the vibrational and rotational constants (except D_v , H_v) are
- (continued on p. 385)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^7\text{Li}^4\text{He}$		$\mu = 2.5486235_2$ $X \ ^2\Sigma (4)(5)(6)$ and $B \ ^2\Sigma (6)$ are unstable except for very small van der Waals minima; $A \ ^2\Pi (3)(6)$ is attractive with an estimated well depth of 500 to 1500 cm^{-1} . Additional excited state potential curves computed by (1)(5). Theoretical coefficients for collision-induced absorption by Li-He ($v = 0 - 300 \text{ cm}^{-1}$) calculated by (4a). The noble-gas broadening of the Li resonance line was studied by (7).							JAN 1977	
$^7\text{Li}^4\text{He}^+$		Theoretical calculations of the ground state potential (2)(3)(9) predict D_e and r_e values varying from 0.064 eV and 1.98 \AA to 0.075 eV and 1.92 \AA , respectively. See also (1)(8)							JAN 1977 A	
$^7\text{Li}^{127}\text{I}$		$\mu = 6.6484410$ $D_0^0 = 3.5_4 \text{ eV}^a$ Peaks in the electron energy loss spectrum at 7.3 and 9.7 eV. Continuous absorption above 28600 cm^{-1} with maxima at 33900 and 45000 cm^{-1} . ^b Diffuse absorption bands from 29146 to 24507 cm^{-1} . ^c							JAN 1977	
A X $^1\Sigma^+$	0	498.1 ₆ (Z)	3.3 ₉ ^d	0.443182 ₀	0.004090 ^e	1.448	2.391924	A \leftarrow X Rot.-vibr. sp. Rotation spectrum Mol. beam rf electric ^f and magn. reson. ^g	(16) (15) (7)(19) (6)(9) (4)(12)(13) (13)(18) (14)	
$(7)\text{Li}^{(39)}\text{K}$		$(\mu = 5.9454387)$							JAN 1977 A	
B X $^1\Sigma^+$	(17578) 0	(130)	H	Fragment				B \leftarrow X, (R) 17539 H Mol. beam rf el. reson. ^b	(1)* (2) (3)	
		(207)	H		(0.265) ^a		(3.27) ^a			

Li^2H (continued):

derived from $\text{A} \rightarrow \text{X}$ fluorescence series extending to $v'' = 20$, i.e. 82% of the dissociation energy (11); the more accurate data for low v'' from (1) are also included, but not the microwave data of (7).

k_{RKR} potential curve (11).

$^{\ell} + 0.0028_7 (v + \frac{1}{2})^2 - 0.000109_6 (v + \frac{1}{2})^3$; see j . From the millimeter wave spectrum (7) obtain $Y_{01} = 4.233107$ and $Y_{11} = -0.091550$ ($v=0,1$ only).

$^m - 0.0066_3 \times 10^{-3} (v + \frac{1}{2}) + 0.00057_5 \times 10^{-3} (v + \frac{1}{2})^2$; $H_v = [2.118 - 0.105(v + \frac{1}{2})] \times 10^{-8}$ (1).

$^n \mu_{\text{el}}(v=0) = 5.8677 \text{ D}$ (5)(8). Hfs constants (5)(8)(13).

$g_J(v=0, J=1) = -0.2767_4 \mu_N$ from the Zeeman sp. (13); a less precise value was earlier obtained (6) by the magnetic resonance method. See also (10).

- (1) Crawford, Jorgensen, PR 47, 358 (1935); 49, 745
- (2) Velasco, CJP 35, 1204 (1957) | (1936).
- (3) Fallon, Vanderslice, Mason, JCP 32, 1453 (1960); 33, 944 (1960) [Erratum].
- (4) Singh, Jain, CJP 40, 520 (1962).
- (5) Wharton, Gold, Klemperer, JCP 37, 2149 (1962).
- (6) Lawrence, Anderson, Ramsey, PR 130, 1865 (1963).
- (7) Pearson, Gordy, PR 177, 59 (1969).
- (8) Rothstein, JCP 50, 1899 (1969).
- (9) Stwalley, Way, Velasco, JCP 60, 3611 (1974).
- (10) Docken, Freeman, JCP 61, 4217 (1974).
- (11) Ennen, Ottinger, CPL 36, 16 (1975).
- (12) Ihle, Wu, JCP 63, 1605 (1975).
- (13) Freeman, Jacobson, Johnson, Ramsey, JCP 63, 2597 (1975).

LiHe , LiHe^+ :

- (1) Schneiderman, Michels, JCP 42, 3706 (1965).
- (2) Catlow, McDowell, Kaufman, Sachs, Chang, JP B 3, 833
- (3) Krauss, Maldonado, Wahl, JCP 54, 4944 (1971). | (1970).
- (4) Dehmer, Wharton, JCP 57, 4821 (1972).
- (4a) Bottcher, Dalgarno, Wright, PR A 7, 1606 (1973).
- (5) Pascale, Vandeplanque, JCP 60, 2278 (1974).
- (6) Bottcher, Cravens, Dalgarno, PRS A 346, 157 (1975).
- (7) Gallagher, PR A 12, 133 (1975).
- (8) Morrison, Akridge, Ellis, Pai, McDaniel, JCP 63, 2238
- (9) Hariharan, Staemmler, CP 15, 409 (1976). | (1975).

LiI : ^aClose agreement between several thermochemical values [(10); mass-spectrom.(5); flame-photom. (11)] and the spectroscopic value of (1).

^bAbsorption cross sections (15). UV absorption in inert matrices (17) shows banded structure in the region 34500 - 40000 cm^{-1} indicating the existence of a stable upper state (possibly lowest excited 0^+) with $\omega_e \approx 365$.

^cA broad single band appears at 28560 cm^{-1} in matrix absorption spectra (17).

^d $\omega_e v_e = +0.08$; vibrational constants from the IR sp.(9).

^e $v_e = +0.000015_3$. For constants of ^6LiI see (13).

^fDipole moments for ^6LiI : $\mu_{\text{el}}(v=0,1) = 7.428_5, 7.512_0 \text{ D}$ (13). Hfs constants (13)(18); see also (4) and (2)(3)(8).

$g_J(^7\text{LiI}) = (+)0.107 \mu_N$. Li NMR spectrum (2)(3)(8).

References on p. 387.

LiK : ^aEstimated constants for $^7\text{Li}^{39}\text{K}$ (3). See also (4).

^b $\mu_{\text{el}}(^7\text{Li}^{39}\text{K}; v=0, J=1) = 3.4_5 \text{ D}$; also values of eqQ.

References on p. 387.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(7) Li(84) Kr B $2\Sigma^+$ A 2Π (13790) X $2\Sigma^+$ 0		$(\mu = 6.4746469)$	$D_e^0 = 0.0084 \text{ eV}^a$							JAN 1977
			Unstable except for a small van der Waals minimum. ^b				3.18^c 4.78^a			
			Attractive potential, $D_e \approx 1185 \text{ cm}^{-1}$. ^c							
			Unstable except for a small van der Waals minimum. ^d							
(7) Li(84) Kr ⁺										JAN 1977
$^7\text{Li } ^{14}\text{N}$										JAN 1977
$^7\text{Li } ^{23}\text{Na}$ B 1Π X 1Σ 0										JAN 1977 A

LiKr, LiKr⁺:

^aFrom high-resolution differential scattering cross sections (3); see also (2).

^bSemiempirical calculations of (1).

^cMorse potential parameters (average of two suggested values) from the analysis of the far-wing fluorescence spectrum longward of the Li resonance line at 14904 cm^{-1} (5). See also (6).

^dSee the potential energy curves in (2)(3)(5).

^eFrom Li⁺-off-Kr differential scattering cross sections (4).

(1) Baylis, JCP 51, 2665 (1969).

(2) Dehmer, Wharton, JCP 57, 4821 (1972).

(3) Auerbach, JCP 60, 4116 (1974).

(4) Böttner, Dimpfl, Ross, Toennies, CPL 32, 197 (1975).

(5) Scheps, Ottinger, York, Gallagher, JCP 63, 2581 (1975).

(6) Scheps, Gallagher, JCP 65, 859 (1976).

- LiN: (1) Dykstra, Pearson, Schaefer, JACS 97, 2321 (1975).
 (2) Jordan, JCP 65, 1214 (1976).

LiNa, LiNa⁺:

- ^aA-type doubling, $\Delta v_{ef} = + 1.95 \times 10^{-4} J(J+1)$.
^b_v: numbering unknown.
^c_e $v_e = - 0.0075$.
^d $\mu_{el}(v=0) = 0.463$ D; quadrupole coupling constants (5), for ⁷Li in disagreement with the value from the magnetic resonance spectrum (4). See also (2)[molecular beam electric deflection] and (9)[ab initio calculation, dipole moment function].
^eTheoretical calculation of (8), confirmed by the elastic Na⁺-on-Li scattering data of (7). Slightly lower values computed by (6) and (1) who give also results for other spectroscopic constants.

LiNa, LiNa⁺ (continued):

- (1) Bertoncini, Das, Wahl, JCP 52, 5112 (1970).
 (2) Dagdigian, Graff, Wharton, JCP 55, 4980 (1971).
 (3) Hessel, PRL 26, 215 (1971).
 (4) Brooks, Anderson, Ramsey, JCP 56, 5193 (1972).
 (5) Graff, Dagdigian, Wharton, JCP 57, 710 (1972).
 (6) Oppenheimer, Bottcher, Dalgarno, CPL 15, 24 (1972).
 (7) von Busch, Hormes, Liesen, CPL 34, 244 (1975).
 (8) Habitz, Schwarz, CPL 34, 248 (1975).
 (9) Rosmus, Meyer, JCP 65, 492 (1976).

- LiI: (1) Beutler, Levi, ZPC B 24, 263 (1934).
 (2) Kusch, PR 75, 887 (1949).
 (3) Logan, Coté, Kusch, PR 86, 280 (1952).
 (4) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
 (5) Friedman, JCP 23, 477 (1955).
 (6) Klemperer, Rice, JCP 26, 618 (1957).
 (7) Berry, Klemperer, JCP 26, 724 (1957).
 (8) Kusch, JCP 30, 52 (1959).
 (9) Klemperer, Norris, Büchler, Emslie, JCP 33, 1534 (1960).

- (10) Brewer, Brackett, CRev 61, 425 (1961).
 (11) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
 (12) Rusk, Gordy, PR 127, 817 (1962).
 (13) Breivogel, Hebert, Street, JCP 42, 1555 (1965).
 (14) Mehran, Brooks, Ramsey, PR 141, 93 (1966).
 (15) Davidovits, Brodhead, JCP 46, 2968 (1967).
 (16) Geiger, Pfeiffer, ZP 208, 105 (1968).
 (17) Oppenheimer, Berry, JCP 54, 5058 (1971).
 (18) Jacobson, Ramsey, JCP 65, 1211 (1976).
 (19) Levi, Dissertation (Berlin, 1934).

- LiK: (1) Walter, Barratt, PRS A 119, 257 (1928).
 (2) Weizel, Kulp, AP(Leipzig) 4, 971 (1930).

- (3) Dagdigian, Wharton, JCP 57, 1487 (1972).
 (4) Cavaliere, Ferrante, Lo Cascio, JCP 62, 4753 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(7)Li(20)Ne B $^2\Sigma$ A $^2\Pi$ X $^2\Sigma$		$(\mu = 5.1934518) \quad D_e^0 = 0.0011 \text{ eV}^a$ Semiempirical interaction potential calculations (1). Broadening of the Li resonance line at 6708 Å (14904 cm^{-1}) by neon (4). Model potential calculation (3); see also (1). 5.05^a							JAN 1977	
$^7\text{Li}^{16}\text{O}$ A $^2\Sigma^+$ (2330) ^c X $^2\Pi_i$ 0 ^d		$\mu = 4.8768325 \quad D_0^0 = 3.49 \text{ eV}^a \quad \text{I.P.} = 8.4_5 \text{ eV}^b$ $(866.7)^c \quad (6.7)^c \quad (1.349)^c \quad (0.0199)^c \quad (1.599)^c$ $(851.5)^{ce} \quad (12.5)^c \quad (1.202)^c \quad (0.0151)^c \quad (1.695)^c$						IR spectrum ^f Mol. beam rf el. reson. ^g	(2)(9) (5)	
(7)Li(85)Rb B (17552) X $^1\Sigma^+$ 0		$(\mu = 6.4805376)$ $(81) \quad \text{H} \quad \text{Fragment}^a$ $(185) \quad \text{H}$						B ← X, 17500 H Mol. beam rf el. reson. ^b	(1)(2) (3)	
(7)Li(132)Xe B $^2\Sigma$ A $^2\Pi$ (13380) X $^2\Sigma$ 0		$(\mu = 6.6616695) \quad D_e^0 = 0.0127 \text{ eV}^a$ Repulsive state except for a small van der Waals minimum. ^b Attractive potential, $D_e \approx 1630 \text{ cm}^{-1}$. ^c Repulsive state except for a small van der Waals minimum. ^d 3.0_6^c 4.80^a							JAN 1977	
(7)Li(132)Xe ⁺		$D_e^0 = 0.51 \text{ eV}^e$							JAN 1977	

LiNe: ^aApproximate constants from total scattering cross sections (2).

- (1) Baylis, JCP 51, 2665 (1969).
- (2) Dehmer, Wharton, JCP 57, 4821 (1972).
- (3) Bottcher, Dalgarno, Wright, PR A 7, 1606 (1973).
- (4) Gallagher, PR A 12, 133 (1975).

LiO: ^aThermochemical value [mass-spectrom.(1)(2)(7), flame photom.(4)].

^bElectron impact appearance potential (7).

^cCI calculation of (6); see also (8).

^d $A_0 = -112.0$, $A_1 = -108$; from the radio frequency spectrum (5). The $^2\Pi$ symmetry of the ground state was originally established by molecular beam electric deflection (3).

^eThe fundamental frequencies in krypton (2) and nitrogen (9) matrices are 745 and 700 cm^{-1} , respectively.

^fIn inert gas matrices.

^g $\mu_{el}(v=0) = 6.84\text{ D}$. The hfs parameters have been re-evaluated by (10).

- (1) Berkowitz, Chupka, Blue, Margrave, JPC 63, 644 (1959).
- (2) White, Seshadri, Dever, Mann, Linevsky, JCP 39, 2463 (1963).
- (3) Berg, Wharton, Klemperer, JCP 43, 2416 (1965).
- (4) Dougherty, Dunn, McEwan, Phillips, CPL 11, 124 (1971).
- (5) Freund, Herbst, Mariella, Klemperer, JCP 56, 1467 (1972).
- (6) Yoshimine, JCP 57, 1108 (1972); Yoshimine, McLean, Liu, JCP 58, 4412 (1973).
- (7) Hildenbrand, JCP 57, 4556 (1972).

LiO (continued):

- (8) Marchetti, Julienne, Krauss, JRNBS A 76, 665 (1972).
- (9) Spiker, Andrews, JCP 58, 702 (1973).
- (10) Veseth, JMS 52, 51 (1976).

LiRb: ^aOnly five bands, four of which have $\Delta v=0$.

^bDipole moment of $^7\text{Li}^85\text{Rb}$: $\mu_{el}(v=0) = 4.0_0\text{ D}$, calculated (3) with $B_0 = 0.218$ estimated from Badger's rule [see, however, (4)]. Quadrupole coupling constants (3).

- (1) Walter, Barratt, PRS A 119, 257 (1928).
- (2) Weizel, Kulp, AP(Leipzig) 4, 971 (1930).
- (3) Dagdigian, Wharton, JCP 57, 1487 (1972).
- (4) Cavaliere, Ferrante, Lo Cascio, JCP 62, 4753 (1975).

LiXe, LiXe⁺:

^aFrom high-resolution differential scattering cross sections (3). See also (2).

^bSemiempirical calculation of (1).

^cMorse potential parameters (average of two suggested values) derived from the far-wing fluorescence spectrum longward of the Li resonance line at 14904 cm^{-1} (5). See also (6).

^dSee the potential curves in (2)(5).

^eFrom Li⁺-on-Xe differential scattering cross sections (4).

- (1) See ref. (1) of LiNe.
- (2) See ref. (2) of LiNe.
- (3) Auerbach, JCP 60, 4116 (1974).
- (4) Böttner, Dimpfl, Ross, Toennies, CPL 32, 197 (1975).
- (5) Scheps, Ottinger, York, Gallagher, JCP 63, 2581 (1975).
- (6) Scheps, Gallagher, JCP 65, 859 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{175}\text{Lu}^{19}\text{F}$										
$\mu = 17.1373091$ $D_0^0 a$										
G $^1\Sigma$	33225.9	599.1	H	2.6				G→X,	33220.1	H (2)
F $^1\Sigma$	25831.8	[555.59]	Z	2.6	H	0.25815	0.00169	F→X,	R 25806.28	Z (2)(3)
E $^1\Pi$	24474.10	543.42	Z	2.28		0.25647 ^b	0.00161	E→X,	R 24439.98	Z (3)
D $^1\Pi$	20047.8	569.7	H	2.5		[0.2592] ^c		D→X,	R 20027.33	Z (2)(3)
C	(18894.1)	605.5	H	2.5				C→(X),	18891.5	H (2)
B $^1\Pi$	16799.9	[576.08]	Z	2.5	H	[0.26241] ^d	0.0016	B→X,	R 16784.52	Z (2)(3)*
A $^1\Sigma$	16164.6 ₆	587.9 ₅	Z	2.58		0.26356	0.00162	A→X,	R 16152.73	Z (3)*
X $^1\Sigma(+)$	0	611.79	Z	2.54		0.26764	0.00156			
$^{175}\text{Lu}^1\text{H}$										
$\mu = 1.00205245$										
H $^1\Pi$		a				[4.5548] ^b [4.5365] ^c	(0.131) ^d 0.135 ₄	[179] ^e [177]	[1.923] ₈	H→X, 23525.00 Z (1)* (2)
G $^1\Sigma$		f				4.546 ₀	0.120 ₆ ^g	178	1.9237	G→X, R 19767.00 Z (1)* (2)
F $^1\Pi$						[4.7025] ^h [4.6496] ^b		[213] ⁱ [171]	[1.897]	F→X, V 18921.49 Z (2)
E $^1\Sigma$						[4.627] ₅ ^h		[200]	[1.9067]	E→X, 17732.92 Z (2)
D $^1\Pi$		j				4.534 ^k 4.518	0.131 0.137	230 ^k [217] ^l	1.928 ₀	D→X, ^m R 17050.1 Z (2)
C $^1\Pi$		n				[4.2306] ^o [4.196] ₅	0.102 ₇	[136] ^o [118] ^p	[1.998]	C→X, R 16721.9 Z (2)
B $^1\Sigma$		q				4.572 ₃	0.117 ₁	195 ^r	1.9182	B→X, 15270.00 Z (2)
A $^1\Pi$		s				[4.8623] [4.467] ₄	0.114 ₉	[690] ^t [195] ^u	[1.90]	A→X, 12988.63 Z (2)
X $^1\Sigma(+)$	0	(1520)	(22)			4.6021	0.099 ₀	169 ^v	1.9119	

LuF: ^aThe dissociation energy was estimated (1) at 5.9 eV.
^b Λ -type doubling, $\Delta v_{fe} = (+)0.00030 \times J(J+1)$.
^c Λ -type doubling, $\Delta v_{fe} = (-)0.0032 \times J(J+1)$.
^d Λ -type doubling, $\Delta v_{fe}(v=0) = (-)0.00060 \times J(J+1)$.
 (1) Zmbov, Margrave, AdC No. 72, 267 (1968).
 (2) D'Incan, Effantin, Bacis, JP B 5, L189 (1972).
 (3) Effantin, Wannous, D'Incan, Athénour, CJP 54, 279 (1976).

Lu¹H: ^a $v_0(1-1) = 23473$, $v_0(2-2) = 23389$.
^be levels.
^cf levels.
^dPerturbation in $v=1$.
^e $D_1 = 183 \times 10^{-6}$; $H_0 = + 0.25 \times 10^{-8}$.
^f $v_0(1-1) = 19696$.
^g $v=1$ perturbed.
^hPerturbations in $v=0$ and 1; constants for $v=1$ could not be determined.
ⁱ $H_0 = - 3 \times 10^{-8}$.
^j $v_0(1-1) = 16918.6$.
^kPerturbation in $v=0$. $H_0 = + 4 \times 10^{-8}$, $H_1 = + 7.6 \times 10^{-8}$.
^l $D_1 = 200 \times 10^{-6}$; $H_0 = + 1.4 \times 10^{-8}$.
^mVery weak system, $J' < 7$ not observed.
ⁿ $v_0(1-1) = 16591.0$.
^oPerturbations in $v=0$ and 1. $H_0 = - 0.9 \times 10^{-8}$.
 Constants for $v=1$ could not be determined.
^p $D_1 = 126 \times 10^{-6}$.
^q $v_0(1-1) = 15173.17$.
^r $H_0 = + 0.9 \times 10^{-8}$.
^s $v_0(1-1) = 12904.32$, $v_0(2-2) = 12810.00$.
^t $H_0 = + 5.0 \times 10^{-7}$.
^u $D_1 = 194 \times 10^{-6}$; $H_0 = - 0.5 \times 10^{-8}$, $H_1 = - 2.4 \times 10^{-8}$.
^v $H_e = + 0.5 \times 10^{-8}$.
 (1) D'Incan, Effantin, Bacis, CJP 50, 1810 (1972).
 (2) Effantin, D'Incan, CJP 51, 1394 (1973).

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{175}\text{Lu}^2\text{H}$										
		$\mu = 1.99117769$				$D_0^0 = (3.4) \text{ eV}$				MAR 1975
H $^1\Pi$	23545.9	1058.6	Z 17.4	2.323 ₆ ^a	0.048 ₄	44.4 ^b	1.908 ₈	H→X,	23535.73 Z	(1)(2)
G $^1\Sigma$	19815.5	1023.6	Z 11.3 ^c	2.272 ₅	0.036 ₂ ^c	42.6 ^c	1.930 ₂	G→X, R	19789.28 Z	(1)(2)
F $^1\Pi$	(18922)	[1072.5 ₃]	Z	2.373 ^d	0.036	[110] ^d	1.889	F→X, V	18923.26 Z	(1)(2)
E $^1\Sigma$	17744	[1033.2 ₆]	Z (15.5) ^e	2.369 ₀	0.049 ₃ ^e	46.4 ^f	1.890 ₄	E→X,	17737.05 Z	(1)(2)
D ($^1\Pi$)								D→X, ^g	17129.1 Z	(1)
C $^1\Pi$	16778.2	997.2	Z 16.2 ^h	2.205 ⁱ	0.038 ^h	46.3 ^h	1.959	C→X, R	16737.64 Z	(1)(2)
B $^1\Sigma$	15306.3	[988.5 ₄]	Z (12.1)	2.268 ₁	0.040 ₀	44.4 ^j	1.932 ₀	B→X, R	15274.59 Z	(1)(2)
A $^1\Pi$								A→X,	13039.9 Z	(1)
X $^1\Sigma^{+}$	0	1075.3 ₅	Z 10.3 ^k	2.320 ₃	0.0356	43.3 ^k	1.910 ₂			
$^{175}\text{Lu}^{16}\text{O}$										
		$\mu = 14.6550016_8$				$D_0^0 = 7.1_9 \text{ eV}^a$				MAR 1975 A
		Two short continua in the red.								
C $^2\Sigma^{+}$	24440	(770)	H (5)	[0.34411] ^b		[0.297]	[1.8283 ₄]	C→X, R	24402.90 Z	(3)
B ($^2\Pi_{3/2}$)	21470	793.0 ^c	H 4.0	[0.3528] ^d			[1.805 ₇]	B→X, R	21445 H	(3)(8)(10)* (1)(2)*(4)* (7)(9)
A ($^2\Pi_{1/2}$)	(19392) ^e	(800)	H (5)					A→X, R	(19370) ^e H	(2)* (3) (4)* (9)
X $^2\Sigma^{+}$	0	842.5 ^c	H 3.1 ₀	[0.35806] ^f	0.0016	[0.255]	1.7904			
$(^{175})\text{Lu}^{(195)}\text{Pt}$										
		$(\mu = 92.205411)$				$D_0^0 = 4.1 \text{ eV}^a$				MAR 1975
$(^{175})\text{Lu}^{(32)}\text{S}$										
		$(\mu = 27.0317641)$				$D_0^0 = 5.1_9 \text{ eV}^a$				MAR 1975
$(^{175})\text{Lu}^{(80)}\text{Se}$										
		$(\mu = 54.856813_5)$				$D_0^0 = 4.2_9 \text{ eV}^a$				MAR 1975
$(^{175})\text{Lu}^{(130)}\text{Te}$										
		$(\mu = 74.548536)$				$D_0^0 = 3.3_3 \text{ eV}^a$				MAR 1975

Lu²H: ^a Λ -type doubling $\Delta v_{ef} = + 0.0052 \times J(J+1) - \dots$.
^b $\beta_e = + 1.4 \times 10^{-6}$; $H_0 = + 3.0 \times 10^{-10}$.
^c $w_{ey_e} = - 0.51$; $\gamma_e = - 0.0018$; $\beta_e = + 1.3 \times 10^{-6}$;
 $H_0 \approx + 2 \times 10^{-10}$. Perturbations by E ¹ Σ ; constants in
the Table are effective values.
^d Λ -type doubling $\Delta v_{fe}(v=1) = + 0.022 \times J(J+1) - \dots$.
 $D_1 = 45 \times 10^{-6}$. Strong perturbations.
^e $v \geq 2$ perturbed by G ¹ Σ . Deperturbed constants for $v=2$
in (2).
^f $\beta_e = + 1.6 \times 10^{-6}$.
^gIdentification uncertain.
^h $w_{ey_e} = + 0.21$, $\gamma_e \approx - 0.0011$, $\beta_e = + 0.63 \times 10^{-6}$; $H_0 =$
 $+ 7.2 \times 10^{-10}$.
ⁱ Λ -type doubling $\Delta v_{fe} = + 0.0100 \times J(J+1) - \dots$.
^j $\beta_e = + 0.4 \times 10^{-6}$.
^k $w_{ey_e} = + 0.034$, $\beta_e = - 0.6 \times 10^{-6}$; $H_e = + 6.0 \times 10^{-10}$.
(1) D'Incan, Effantin, Bacis, JP B 5, L187 (1972).
(2) Effantin, d'Incan, CJP 52, 523 (1974).

LuO ^aThermochemical value (mass-spectrom.)(5), recalc. (6).
^bLarge spin doubling, $\gamma_0 = (-)0.4940$. $v=0$ perturbed for
 $N > 30$.
^cRecalculated using bandheads of the B-X 0-0 and 1-0
sequences only.
^d B_v appears to depend irregularly on v ; see (9).
^eFrom (9). The vibrational numbering in (3) differs by
-1 in both upper and lower state leading to $v_{00} \approx 19332$.
^fLarge hyperfine splitting, $4b = 0.663 \text{ cm}^{-1}$ (10).

LuO (continued):

- (1) Watson, Meggers, JRNBS 20, 125 (1938).
- (2) Gatterer, RS 1, 153 (1942).
- (3) Gatterer, Krishnamurty, PPS A 65, 151 (1952).
- (4) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (5) Ames, Walsh, White, JPC 71, 2707 (1967).
- (6) Smoes, Coppens, Bergman, Drowart, TFS 65, 682
(1969).
- (7) Suárez, JP B 3, 1389 (1970).
- (8) Bacis, Bernard, d'Incan, CR B 273, 272 (1971).
- (9) Effantin, Bacis, d'Incan, CR B 273, 605 (1971).
- (10) Bacis, Bernard, CJP 51, 648 (1973).

LuPt: ^aThermochemical value (mass-spectrom.)(1).

- (1) Gingerich, HTS 3, 415 (1971).

LuS: ^aThermochemical value (mass-spectrom.)(1); recal-
culated (2).

- (1) See ref. (6) of LuO.
- (2) Bergman, Coppens, Drowart, Smoes, TFS 66, 800
(1970).

LuSe, LuTe:

^aThermochemical value (mass-spectrom.)(1).

- (1) See ref. (2) of LuS.

Mg₂: ^aFrom the convergence of the vibrational levels v=0...12 of the ground state (4) including the slight extension (v=13) and correction by (9).
^bLowest observed level, vibrational numbering uncertain.
^c $w_{e'}y_e = + 0.001772$. Vibrational numbering established by the observed ²⁴Mg₂ - ²⁶Mg₂ isotope shifts (4).
^d $y_e = + 0.1474 \times 10^{-5}$.
^e $H_e = + 0.23 \times 10^{-11}$.
^fFranck-Condon factors and their dependence on rotation (8).
^gObserved in Kr and Xe matrices by (6) and in Ne, Ar, N₂ matrices by (11). The same authors also observe other absorptions probably related to B-X and C-X in the gas.
^h $w_{e'}y_e = + 0.01624$, $w_{e'}z_e = - 0.000611$.
ⁱ $+ 0.0001068(v+\frac{1}{2})^2 - 0.00000968(v+\frac{1}{2})^3$.
^j $- 0.031 \times 10^{-6}(v+\frac{1}{2}) + 0.021 \times 10^{-6}(v+\frac{1}{2})^2$;
 $H_v = - 0.26 \times 10^{-10} - 0.085 \times 10^{-10}(v+\frac{1}{2})$.
^kTerm values of ro-vibrational levels, RKR potential functions (4)(9). For other potential functions see (7)(10).
^lLong-range potential studied by (5)(9).
 (1) Hamada, PM (7) 12, 50 (1931).
 (2) Weniger, JP(Paris) 25, 946 (1964).
 (3) Edelhoff, Kusch, Lochte-Holtgreven, RRP 13, 125 (1968).
 (4) Balfour, Douglas, CJP 48, 901 (1970).
 (5) Stwalley, JCP 54, 4517 (1971).
 (6) Brewer, Wang, JMS 40, 95 (1971).
 (7) Brett, Chan, CJP 50, 1587 (1972).
 (8) Balfour, Whitlock, CJP 50, 1648 (1972).
 (9) Li, Stwalley, JCP 59, 4423 (1973).
 (10) Muhlhausen, Konowalow, CP 7, 143 (1975).
 (11) Knight, Ebener, JMS 61, 412 (1976).

MgBr: ^aFrom the predissociation in A ²Π.
^bPartial rotational analysis of the 0-0 band (4).
^cPredissociation above v=3.
 (1) Olmsted, ZWP 4, 293 (1906).
 (2) Morgan, PR 50, 603 (1936).
 (3) Harrington, Dissertation (U. of California, 1942).
 (4) Patel, Patel, JP B 2, 515 (1969).
 (5) Reddy, Rao, CS 32 (22), 509 (1970).
 (6) Puri, Mohan, CS 42, 442 (1974).
 MgCl: ^aThermochemical value (mass-spectrom.); average of three reactions (8)(9).
^bNo clear identification of the various isotopic band heads was possible.
^c $w_{e'}y_e = - 0.025$.
^dThe assignment of the emission band heads by (2) is not correct.
^eFrom (5). Somewhat different results in (7).
 (1) Querbach, ZP 60, 109 (1930).
 (2) Parker, PR 47, 349 (1935).
 (3) Morgan, PR 50, 603 (1936).
 (4) Harrington, Dissertation (U. of California, 1942).
 (5) Morgan, Barrow, Nature 192, 1182 (1961).
 (6) Rao, Rao, IJP 37, 640 (1963).
 (7) Patel, Patel, IJP 42, 254 (1968).
 (8) Hildenbrand, JCP 52, 5751 (1970).
 (9) Farber, Srivastava, CPL 42, 567 (1976).
 MgCs: (1) Barratt, PRS A 109, 194 (1925).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References		
								Design.	v_{00}			
$^{24}\text{Mg}^{19}\text{F}$		$\mu = 10.6012334$ $D_0^0 = 4.75 \text{ eV}^a$ (V shaded emission bands in the region 1800 - 1900 \AA , attributed to MgF^+ by (15), are due to the $B \rightarrow X$ transition of AlF .)								MAR 1977		
G ($^2\Sigma$)	74304.2	800.0	H	6.18	} Four 0-0 sequences; no details.			G \leftrightarrow X, (V)	74343	(15)		
F ($^2\Sigma$)	57067.2	756.6	H	4.06				F \leftrightarrow X, (V)	57085	(15)		
E ($^2\Pi$)	55694.9	775.9	H	4.00				E \leftrightarrow X, (V)	55722	(15)		
D ($^2\Pi$)	54263.6	792.3	H	4.38				D \leftrightarrow X, (V)	54299	(15)		
C $^2\Sigma^+$	42538.9	[813.10]	Z	(5.04)		0.55102	0.00449	[0.00991] ^b	1.6988	C \leftarrow X, ^c V	42589.64 Z	(3)* (6)
B $^2\Sigma^+$	37167.3	[750.94]	Z	(5.60)		0.53844	0.00510	[0.01083] ^d	1.7185	B \leftrightarrow X, ^e V	37187.45 Z	(1)(2)* (3)* (6)
A $^2\Pi_r$	27851.2 f	746.0	H	3.97		0.52105 ^g	0.00327	[0.0038] ^h	1.7469	A \leftrightarrow X, ⁱ V	27863.7 Z	(2)* (3)* (6)
	27816.1	[740.12]	Z								27829.60 Z	
X $^2\Sigma^+$	0	[711.69]	Z	(4.94)		0.51922	0.00470	[0.01080] ^j	1.7500	ESR sp. ^k		(14)
$^{24}\text{Mg}^1\text{H}$		$\mu = 0.96718516$ $D_0^0 = 1.34 \text{ eV}^a$ Unidentified line structure at 42570 cm^{-1} [em. and abs., (2)(3)(8)(10)] and $43180 - 43520 \text{ cm}^{-1}$ [abs., (12)].								MAR 1977		
I ($^2\Pi$)				[5.96]		[2]	[1.71 ₀]	I \leftarrow X, V	47997.6 Z	(12)		
H ($^2\Sigma^+$)					R shaded band with head at 2100 \AA .			H \leftarrow X, R	47543 (Z)	(12)		
G ($^2\Sigma^+$)					V shaded band with head at 2172 \AA .			G \leftarrow X, V	46082 (Z)	(12)		
D $^2\Sigma^-$	(42065)	(1630) ^b		[6.296] ^c		[3.8]	[1.664]	D \rightarrow A, V	22861.5 ^d	(6)(10)		
C $^2\Pi(r)$	(41164) ^e	[1623.4] Z		6.161 ^f	0.144	3.0	1.682	C \rightarrow A, V	21956.5 ^d	(1)(2)(7)(10)		
								C \leftrightarrow X, V	41235.9 Z	(1)* (3)(4) (7)(8)(10) (17)*		
E $^2\Sigma^+$	(35568)	[1444.8] Z	^g		6.23	0.30 ^h	[3.3] ⁱ	E \leftarrow X, V _R	35550.6 Z	(11)(13)* (20)		
B' $^2\Sigma^+$	22410.5	828.0 Z	11.6 ^j	[2.596]	^k	1.2 ^l	2.597	B' \rightarrow X, R	22081.9 Z	(20)(22)		

MgF: ^aThermochemical value (mass-spectrom.)(7); similar results can be obtained from (4) and (5) with the use of appropriately revised auxiliary data.

^b $D_1 = 0.00984 \times 10^{-4}$.

^cFranck-Condon factors (8)(11).

^d $D_1 = 0.01085 \times 10^{-4}$.

^eFranck-Condon factors (8)(12).

^f $A = +37$ (6)(13). The regular character of this state is suggested by the theoretical calculations of (9) (13) and supported by the analysis of the ESR sp.(14).

^gFor Λ -type doubling constants see (6) and (13).

^h $D_1 = 0.0078 \times 10^{-4}$.

ⁱMorse potential Franck-Condon factors (10).

^j $D_1 = 0.01075 \times 10^{-4}$.

^kIn Ne and Ar matrices at 4K.

- (1) Jevons, PRS A 122, 211 (1929).
- (2) Jenkins, Grinfeld, PR 45, 229 (1934).
- (3) Fowler, PR 59, 645 (1941).
- (4) Ehlert, Blue, Green, Margrave, JCP 41, 2250 (1964).
- (5) Murad, Hildenbrand, Main, JCP 45, 263 (1966).
- (6) Barrow, Beale, PPS 91, 483 (1967).
- (7) Hildenbrand, JCP 48, 3657 (1968).
- (8) Maheshwari, Singh, Shukla, JP B 1, 993 (1968).
- (9) Walker, Richards, JP B 1, 1061 (1968).
- (10) Singh, Shukla, Maheshwari, JQSRT 9, 533 (1969).
- (11) Rao, Lakshman, JQSRT 10, 945 (1970).
- (12) Rao, Lakshman, Physica 46, 609 (1970).
- (13) Walker, Richards, JP B 3, 271 (1970).
- (14) Knight, Easley, Weltner, Wilson, JCP 54, 322 (1971).
- (15) Novikov, Gurvich, JAS 14, 820 (1971).

Mg¹H: ^aFrom extrapolations of the vibrational levels in X, A, and B'. Close agreement with the theoretical value of (21), $D_0 = 1.25$ eV.

^bEstimated from $\omega^2 = 4B^3/D$ and from the observed isotope shift of the 0-0 band.

^cSpin doubling, $|y| = 0.01$.

^dAverage of the two subband origins (10).

^e $A_0 = (+)3.7$; (17) gives -3.7 but his arguments are not conclusive.

^fThe P and R branches of the C \rightarrow X, 0-0 band break off above $N'=10$; bands with $v' > 0$ have Q branches only. The predissociation is caused by B' $^2\Sigma^+$; see (20).

^g $\Delta G(3/2) = 1490$. The $v=2$ level was formerly believed to be $v=0$ of a new $^2\Sigma$ state (B $^2\Sigma^+$), see (4)(5)(9)(10). Similarly, (11) assigned the 1-0 band as 0-0 band of a new system F \leftarrow X.

^h B_2 (see ^g) = 5.44_8 . Transitions to $v=1$ are discrete but those to $v=2$ are diffuse indicating that the state causing the predissociation [B' $^2\Sigma^+$, see (20)] crosses the E state potential curve between $v=1$ and 2. Emission from $v=2$ has been observed at high pressure.

ⁱ $D_1 = 4.0 \times 10^{-4}$; $D_2 = 2.7_1 \times 10^{-4}$, $H_2 = +8.6 \times 10^{-8}$ (see ^g).

^jThe equilibrium constants in (22) do not reproduce the observed intervals, probably owing to an error in $\omega_e z_e$.

$D_e \approx 10900 \text{ cm}^{-1}$ (22).

^k $B_v(v=1,2,3,4\dots 9) = 2.605, 2.618, 2.608, 2.592 \dots 2.419$; $B_e = 2.585$, but the higher order constants of (22) do not reproduce their data. Small perturbations by A $^2\Pi$. RKR potential curve (22). See also (24).

^l $\beta_e \approx 0.13 \times 10^{-4}$.

(continued on p. 398)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{24}\text{Mg}^1\text{H}$ (continued)										
A $^2\Pi_r$	19226. ₈ ^m	1598.17	Z 31.08 ₅ ⁿ	6.1913	0.1931 ^o	3.60 ^p	1.6778	A \leftrightarrow X, ^{qr} v	19278. ₄ ^d	(6)(10)(16) (17)(23)
X $^2\Sigma^+$	0	1495.20	Z 31.889 ^s	5.8257	0.1859 ^t	3.44 ^p	1.7297	ESR sp. ^u		(19)
$^{24}\text{Mg}^2\text{H}$										MAR 1977
		$\mu = 1.85807372$		$D_0^0 = 1.36 \text{ eV}^a$						
G $^2\Sigma^+$				[3.26] ^b		[0.8]	[1.66 ₈]	G \rightarrow X, v	46071.4	Z (6)
D $^2\Sigma^-$	(42080)	(1180) ^c		[3.27 ₃]		[1.0]	[1.665]	D \rightarrow A, v	22860. ₀	Z (4)
C $^2\Pi(r)$	(41180)	[1140.1]	Z	3.256 ^{de}	0.073	0.92	1.669	C \rightarrow A, v	21940 ^f	(4)
		h		[3.20]	h		[1.68 ₄]	C \leftrightarrow X, v	41214.2 ^g	Z (1)(3)(4)(8)
E $^2\Sigma^+$								E \leftarrow X, ^v R	35549.0	Z (5)*
B' $^2\Sigma^+$	22410. ₃	597. ₅	Z 6.0 ₅ ⁱ	[1.350]	j	0.25 ^k	2.596	B' \rightarrow X, ^l R	22172. ₇	Z (10)
A $^2\Pi_r$	19235. ₅ ^m	1154.75	Z 16.67 ₅ ⁿ	3.2190	0.0679 ₅ ^o	0.964 ^p	1.6788	A \leftrightarrow X, v	19273.7 ₁ ^g	Z (2)* (8)(9)
X $^2\Sigma^+$	0	1077.8 ₉	Z 16.1 ₂ ^q	3.0306	0.06289 ^r	0.92 ₁ ^s	1.7302			

Mg^1H (continued):

$^m A_0 = + 35.3$ (17).

$^n w_e y_e = - 0.633$. These constants (for $v \leq 3$) have been recalculated from the three ΔG values obtained by (23); the equilibrium constants determined by (23) do not reproduce their data. $D_e \approx 14200 \text{ cm}^{-1}$ (23).

$^o y_e = + 0.0005$. Small perturbations by B' $2\Sigma^+$.

$^p D_v$ increases rapidly with v.

q Oscillator strength $f_{00} = 0.257$ [see (23) and references given there], much larger than the earlier experimental value of (14).

r (16) has measured the 0-0 and 0-1 bands of ^{25}MgH and ^{26}MgH ; see also (15)(18).

$^s w_e y_e = + 0.384$, $w_e z_e = - 0.113$ (23); $D_e^0 \approx 11700 \text{ cm}^{-1}$ (23). $^t + 0.0039_3(v+\frac{1}{2})^2 - 0.0012_3(v+\frac{1}{2})^3$. The last term was not reported by (23) but must be included for a satisfactory fit to their data ($v=0\ldots 6$).

u In Ar matrices at 4K.

(1) Pearse, PRS A 122, 442 (1929).

(2) Guntzsch, ZP 87, 312 (1934).

Mg¹H (continued):

- (3) Guntzsch, ZP 93, 534 (1935).
- (4) Grundström, Dissertation (Stockholm, 1936).
- (5) Grundström, Nature 137, 108 (1936).
- (6) Guntzsch, ZP 104, 584 (1937).
- (7) Guntzsch, ZP 107, 420 (1937).
- (8) Turner, Harris, PR 52, 626 (1937).
- (9) Guntzsch, ZP 110, 549 (1938).
- (10) Guntzsch, Dissertation (Stockholm, 1939).
- (11) Khan, PPS 77, 1133 (1961).
- (12) Khan, PPS 80, 209 (1962).
- (13) Khan, PPS 82, 572 (1963).
- (14) Main, Carlson, DuPuis, JQSRT 7, 805 (1967).
- (15) Branch, ApJ 159, 39 (1970).
- (16) Balfour, ApJ 162, 1031 (1970).
- (17) Balfour, JP B 3, 1749 (1970).
- (18) Boyer, AA 12, 464 (1971).
- (19) Knight, Weltner, JCP 54, 3875 (1971).
- (20) Balfour, Cartwright, CPL 32, 82 (1975).
- (21) Meyer, Rosmus, JCP 63, 2356 (1975).
- (22) Balfour, Cartwright, CJP 54, 1898 (1976).
- (23) Balfour, Cartwright, AA(Suppl.) 26, 389 (1976).
- (24) Sink, Bandrauk, Henneker, Lefebvre-Brion, Raseev, CPL 39, 505 (1976).

- Mg²H: ^aFrom the value for Mg¹H, in good agreement with an extrapolation of the ground state vibrational levels.
- ^bR branch breaks off at N'=12.
- ^cSee ^b of Mg¹H.
- ^dB(R,P) - B(Q) \approx + 0.008.
- ^e(4) reports breaking-off of P and R branches in the C \rightarrow X, 0-0 band above N'=14. No line broadening is observed in the absorption spectrum (8).

Mg²H (continued):

- ^fSee ^d of Mg¹H.
- ^gRefers in the upper state to the zero point of the Hill-Van Vleck equation.
- ^hFragments of what is probably the E \leftarrow X, 1-0 band have been found (?) between 36690 and 36930 cm⁻¹. Two additional levels, formerly attributed to a separate ² Σ^+ state (B ² Σ), have been identified at 39593.8 cm⁻¹ [in emission (4) and absorption (7), B_v = 2.862] and at 38330.3 cm⁻¹ [in absorption (7), B_{v-1} = 2.915].
- ⁱD_e \approx 11200 cm⁻¹ (10).
- ^jB_v(v=1,2,4,5,6) = 1.355, 1.359, 1.358, 1.354, 1.346; B_e = 1.346. No emission from v'=3 has been found. Small perturbations by A ² Π .
- ^k $\beta_e \approx$ + 0.04₃ x 10⁻⁴.
- ^lRKR Franck-Condon factors (10).
- ^mA₀ = + 35.0₄, A₁ = 36.1, A₂ = 36.7.
- ⁿw_ey_e = - 0.183₃; D_e \approx 15500 cm⁻¹ (9).
- ^oy_e = - 0.00122₅. Small perturbations by B' ² Σ .
- ^p $\beta_e =$ + 0.008₉ x 10⁻⁴.
- ^qw_ey_e = + 0.08₅, w_ez_e = - 0.029₃; 4th-order fit to the ΔG values of (9) whose equilibrium constants do not satisfactorily reproduce their data. D_e⁰ \approx 11500 cm⁻¹ (9).
- ^ry_e = - 0.00144.
- ^s+ 0.012 x 10⁻⁴(v+ $\frac{1}{2}$) + ...
- (1) See ref. (3) of Mg¹H.
 - (2) Fujioka, Tanaka, Sci. Pap. IPCR (Tokyo) 30, 121 (1936).
 - (3) See ref. (8) of Mg¹H.
 - (4)...(7) See ref. (10)...(13) of Mg¹H, respectively.
 - (8) See ref. (17) of Mg¹H.
 - (9) Balfour, Cartwright, CJP 53, 1477 (1975).
 - (10) See ref. (22) of Mg¹H.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{24}\text{Mg}^1\text{H}^+$		$D_0^0 = (2.08) \text{ eV}^a$							MAR 1977	
B $^1\Pi$	50476	[527.3]	Z	[3.380] ^b	0.283	[4.7] ^c	[2.271]	B \rightarrow X, ^d R	49898.6 Z	(3)(5)(8)
A $^1\Sigma^+$	35904.52	1135.8	Z 8.18 ₁ ^e	4.3295	0.0680 ₃ ^f	2.510 ^g	2.0064	A \rightarrow X, ^{dh} R	35628.81 Z	(1)(2)(5)(7)(8)*
X $^1\Sigma^+$	0	1699.1	Z 31.93 ₅ ⁱ	6.3870	0.1819 ₄ ^j	3.664 ^k	1.6519			
$(^{24})\text{Mg}^2\text{H}^+$		$D_0^0 = (2.1_1) \text{ eV}^l$							MAR 1977	
A $^1\Sigma^+$	35902.6	817.0	Z 3.47 ^m	2.252	0.024 ₃ ⁿ	0.64	2.007	A \rightarrow X, R	35701.0 Z	(4)(6)
X $^1\Sigma^+$	0	1226.6	Z 16.30 ^o	3.324	0.066 ₇ ^p	0.96	1.652			
$(^{24})\text{Mg}^{127}\text{I}$		$(\mu = 20.1724379) \quad D_0^0 = (2.9_2) \text{ eV}^a$							MAR 1977	
D	26680	295	H 0.5					D \rightarrow X,	26670 H	(3)
C	26099	270	H 0.72					C \rightarrow X,	26076 H	(3)
B	25612	295	H					B \leftrightarrow X R	25602 H	(1)(3)
A	24319	323	H 1.0					A \leftrightarrow X, V	24322 H	(1)(3)
X ($^2\Sigma$)	0	316	H 0.50							
$(^{24})\text{Mg}^{(39)}\text{K}$ $(^{24})\text{Mg}^{23}\text{Na}$ $(^{24})\text{Mg}^{(85)}\text{Rb}$		$(\mu = 14.8461445)$ One R shaded and two V shaded absorption bands at 15264 and 19411, 21678 cm^{-1} . $(\mu = 11.7384318)$ V shaded absorption band at 18895 cm^{-1} . $(\mu = 18.7022250)$ V shaded absorption band at 21144 cm^{-1} .								APR 1978
										(1)*

Mg¹H⁺, Mg²H⁺;

^aExtrapolation of vibrational levels in X ¹Σ and A ¹Σ.

^bB(R,P) - B(Q) = + 0.004.

^cH₀ = - 8 x 10⁻⁸.

^dThe spectra of the isotopes ²⁵Mg¹H⁺ and ²⁶Mg¹H⁺ have also been analyzed (8).

^eω_ey_e = - 0.147₉, ω_ez_e = - 0.0078₈; D_e ≈ 18000 cm⁻¹.

^f+ 0.000039₈(v+½)² - 0.0001208(v+½)³. RKR potential curve (8).

^gH_e = + 1.82 x 10⁻⁸; higher order constants in (8).

^hRKR Franck-Condon factors (8).

ⁱω_ey_e = - 0.188₂, ω_ez_e = - 0.0204₄; D_e⁰ ≈ 17000 cm⁻¹.

^j+ 0.00020₂(v+½)² - 0.00062₉(v+½)³ + 0.000045₇(v+½)⁴ - 0.000002₅(v+½)⁵. RKR potential curve (8).

^kH_e = + 2.07 x 10⁻⁸; higher order terms in (8).

^lFrom the value for Mg¹H⁺.

^mω_ey_e = - 0.11₇.

ⁿγ_e = - 0.0003; from the average B_v values of (4)(6).

^oω_ey_e = - 0.16₇.

^pγ_e = - 0.0009; see ⁿ.

(1) Pearse, PRS A 125, 157 (1929).

(2) Guntzsch, ZP 87, 312 (1934).

(3) Guntzsch, ZP 107, 420 (1937).

(4) Juraszyska, Szulc, APP 7, 49 (1938).

(5) Guntzsch, Dissertation (Stockholm, 1939).

(6) Guntzsch, AMAF A 31, No. 22 (1945).

(7) Pillow, PPS A 62, 237 (1949).

(8) Balfour, CJP 50, 1082 (1972).

MgI: ^aFrom an ill-defined threshold for dissociative photo-ionization, and from the heat of atomization of MgI₂, using an assumed value for the ionization potential of MgI (2).

(1) Morgan, PR 50, 603 (1936).

(2) Berkowitz, Chupka, JCP 45, 1287 (1966).

(3) Puri, Mohan, Pramāṇa 4, 171 (1975).

MgK, MgNa, MgRb:

(1) Barratt, PRS A 109, 194 (1925).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{24}\text{Mg}^{16}\text{O}$										
		$\mu = 9.5957762_8$ $D_0^0 = (3.5_3) \text{ eV}^a$								MAR 1977 A
G 1_{Π}	[40259.8]			[0.5224] ^b		[2.27]	[1.834]	G \rightarrow A, V	36365.4 Z	(22)*
F 1_{Π}	(37922)	[696] H		[0.5590] ^c		[1.424]	[1.7728]	G \rightarrow X, R	39868.6 Z	(22)*
E 1_{Σ^+}	(37722)	[705] ^d H		[0.5249] ^b		[1.14]	[1.829]	F \rightarrow X, R	37879.1 Z	(21)*
C 1_{Σ^-}	30080.6	632.4 Z	5.2	0.5008	0.0048	[1.27] ^e	1.8729	E \rightarrow A, V	34180 H ^Q	(27)*
e 3_{Σ^-}		Very weakly bound or repulsive state; see (19). Continuous absorption above 31250 cm^{-1} by shock-heated MgO in Ar/O ₂ mixtures.								(18)* (25)*
D 1_{Δ}	29851.6	632.5 Z	5.3	0.5014	0.0048	[1.26] ^g	1.8718	C \rightarrow A, ^f R	26500.94 Z	(4)* (10)
d 3_{Δ_i}	(29300) ⁱ	(650)		(0.50)			(1.87)	(e \leftarrow a)		(23)
c 3_{Σ^+}	(28300)	The assignment of the bands to MgO is still uncertain. See also (19).								(10)
B 1_{Σ^+}	19984.0	824.08 Z	4.76 ^j	0.5822 ^k	0.0045	1.14 ^l	1.7371	D \rightarrow A, ^{fh} R	26272.04 Z	(1b)(23)(26)
A 1_{Π}	3563.3	664.44 Z	3.91	0.5056 ^o	0.0046	1.18	1.8640	d \leftrightarrow a, (V)	26867 H ^Q	(23)
a 3_{Π_i}	(2400) ^p	(650)		(0.50)			(1.87)	(c \leftarrow a)	25900	(1a)*
X 1_{Σ^+}	0	785.06 Z	5.18	0.5743 ^k	0.0050	1.22 ^q	1.7490	B \rightarrow A, ^m V	16500.29 Z	(1)(1a)(3)*
								B \leftrightarrow X, ⁿ V	20003.57 Z	
								r		
$^{24}\text{Mg}^{32}\text{S}$										
		$\mu = 13.7042725$ $D_0^0 \leq 2.4 \text{ eV}^a$								MAR 1977
B 1_{Σ^+}	23052.59	497.34 Z	2.333	0.25518	0.00155	0.269	2.1956	B \leftrightarrow X, R	23036.98 Z	(1)(4)*
X 1_{Σ^+}	0	528.74 Z	2.704	0.26797	0.00176	0.276	2.1425			

For MgRb see p. 400.

MgO: ^aThe dissociation energy (to Mg ¹S + O ³P) is quite uncertain. The value given is the thermochemical value of (6) as corrected (19) for the presence of the low-lying a³Π state. From flame photometry (15) obtain 4.1₆ eV assuming a ³Σ ground state, while (2) also from flame photometry but assuming a ¹Σ ground state obtain 4.3₄ eV.

^bSeveral rotational perturbations.

^cSmall Λ-type doubling; intensity perturbations.

^dData for Mg¹⁸O are given by (25).

^eD₁ = 1.30 × 10⁻⁶; H₀ = 0.48 × 10⁻¹¹.

^fFranck-Condon factors (12)(17)(24).

^gD₁ = 1.29 × 10⁻⁶.

^hFor ¹⁸O - ¹⁶O isotope shifts see (10).

ⁱA ≈ - 25.

^jVibrational isotope shifts for ²⁴Mg¹⁸O and ²⁶Mg¹⁶O (8).

^kRKR potential functions (13).

^lβ_e = + 0.02₅ × 10⁻⁶.

^mFranck-Condon factors (5); oscillator strength (11)(16).

ⁿObserved in absorption in shock-heated Ar/O₂ mixtures containing MgO (23). Franck-Condon factors (5)(7)(9); oscillator strength (11)(16); dependence of transition moment on r from measured intensities (20).

^oSmall Λ-type doubling.

^pA ≈ - 50; T_e is the theoretical value of (19). An experimental value of 3200 ± 1000 is given by (23).

^qβ_e = + 0.02 × 10⁻⁶.

^rTheoretical ground state properties (14); more recent calculations of ground and excited states (19).

(1) Lagerqvist, AMAF A 29, No. 25 (1943).

(1a) Lagerqvist, Uhler, AF 1, 459 (1949).

(1b) Brewer, Porter, JCP 22, 1867 (1954).

(2) Veits, Gurvich, OS 1, 22 (1956); ZFK 31, 2306 (1957).

MgO (continued):

- (3) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (4) Brewer, Trajmar, Berg, ApJ 135, 955 (1962).
- (5) Nicholls, JRNBS A 66, 227 (1962).
- (6) Drowart, Exsteen, Verhaegen, TFS 60, 1920 (1964).
- (7) Ortenberg, Glasko, Dmitriev, SAAJ 8, 258 (1964).
- (8) Pešić, PPS 83, 885 (1964).
- (9) Prasad, PPS 85, 810 (1965).
- (10) Trajmar, Ewing, ApJ 142, 77 (1965).
- (11) Main, Carlson, DuPuis, JQSRT 7, 805 (1967).
- (12) Srivastava, Maheshwari, PPS 90, 1177 (1967).
- (13) Thakur, Singh, JSRBHU 18, 253 (1967).
- (14) Yoshimine, JPSJ 25, 1100 (1968).
- (15) Cotton, Jenkins, TFS 65, 376 (1969).
- (16) Main, Schadee, JQSRT 9, 713 (1969).
- (17) Gandara, Schamps, Bécart, CR B 270, 1213 (1970).
- (18) Singh, JP B 4, 565 (1971).
- (19) Schamps, Lefebvre-Brion, JCP 56, 573 (1972).
- (20) Dube, IJPAP 11, 445 (1973).
- (21) Singh, JP B 6, 1339 (1973).
- (22) Singh, JP B 6, 1917 (1973).
- (23) Evans, Mackie, CP 5, 277 (1974).
- (24) Shadrin, Zhirnov, OS(Engl. Transl.) 38, 367 (1975).
- (25) Antić-Jovanović, Pešić, Bojović, JMS 60, 416 (1976).
- (26) Schamps, Gandara, JMS 62, 80 (1976).
- (27) Antić-Jovanović, Bojović, Pešić, JP B 9, L575 (1976).

MgS: ^aFrom mass-spectrometric studies (2)(3).

- (1) Wilhelm, Iowa State Coll. J. Sci. 6, 475 (1932).
- (2) Colin, ICB 26, No. 9 (1961).
- (3) Colin, Goldfinger, Jeunehomme, TFS 60, 306 (1964).
- (4) Marcano, Barrow, TFS 66, 2936 (1970).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{55}\text{Mn}_2$		$\mu = 27.469023_2$ $D_0^0 = 0.2_3 \text{ eV}^a$ Absorption in the region $14400 - 16500 \text{ cm}^{-1}$; in Ar matrices at 10 K. $w' \approx 111$.								MAR 1976 (2)
$^{55}\text{Mn}^{79}\text{Br}$		$\mu = 32.390081_4$ $D_0^0 = 3.2_2 \text{ eV}^a$ Bands in the region $15800 - 16400 \text{ cm}^{-1}$, attributed to MnBr by (6), are probably due to CaBr. Emission bands in the visible and near infrared: $v_e = 20024.6$; $w'_e = 286.6$, $w'_e x'_e = 1.4$; $w''_e = 295.9$, $w''_e x''_e = 1.6$; $v_e = 10682.1$; $w'_e = 290.4$, $w'_e x'_e = 0.13$; $w''_e = 291.3$, $w''_e x''_e = 0.01$; $v_e = 10667.5$; $w'_e = 295.6$, $w'_e x'_e = 0.62$; $w''_e = 298.8$, $w''_e x''_e = 0.61$;								MAR 1975 (10)
A ($^7\Pi$)	26303.7 ^f	302.3	H ^{Q4} 0.6					b	R 20020.0 H ^{Q5}	(8)*
X ($^7\Sigma$)	0	286.7	H ^{Q4} 0.8					c	R 19705.9 H ^Q 19669.8	(8)*
								d	R 10681.6 H ^Q	(7)*
								e	R 10665.9 H	(7)*
								A \leftrightarrow X, V	26311.6 H ^{Q4}	(1)(2)(3)* (4)(5)
$^{55}\text{Mn}^{(35)}\text{Cl}$		$(\mu = 21.3678872)$ $D_0^0 = 3.7_0 \text{ eV}^a$ Emission bands in the visible and near infrared: $v_e = 20115$; $w'_e = 378$, $w''_e = 386$, $w''_e x''_e = 386$, $v_e = (19938)$; $w'_e = (385)$, $w''_e = (410)$, $w''_e x''_e = (410)$, $v_e = 11420$; $w'_e = 385$, $w''_e = 398$, $w''_e x''_e = 398$;								MAR 1975
B ($^7\Sigma$)	40807	[320]	H					c	R 20111 H ^Q	(8)*
A ($^7\Pi$)	27005.0 ^f	[407.9]	H	g				d	R (19925)	(8)*
X ($^7\Sigma$)	0	[382.4]	H	g				e	R 11414 H ^Q	(7)*
								B \leftarrow X, V	40776 H	(4)
								A \leftrightarrow X, V	27017.8 H ^{Q4}	(1)(2)(3) (4)* (5)(6)

Mn₂: ^aThermochemical value (mass-spectrom.)(1).
 (1) Kant, Lin, Strauss, JCP 42, 1983 (1968).
 (2) De Vore, Ewing, Franzen, Calder, CPL 35, 78 (1975).

MnBr: ^aThermochemical value (flame photometry)(9).
^bQ, R, S heads; possibly quintet system.
^cTwo sequences of double headed bands.
^dQ, R heads; possibly additional branches.
^eSingle heads.
^f|A| \approx 58.
 (1) Mesnage, AP(Paris) 12, 5 (1939).
 (2) Müller, HPA 16, 3 (1943).
 (3) Bacher, HPA 21, 379 (1948).
 (4) Rao, IJP 23, 517 (1949).
 (5) Hayes, Nevin, PRIA A 52, 15 (1955).
 (6) Hayes, Nevin, PPS A 68, 665 (1955).
 (7) Hayes, PPS A 68, 670 (1955).
 (8) Hayes, PPS A 68, 1097 (1955).
 (9) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
 (10) Barrow, in DONNSPEC (1970).

MnCl: ^aThermochemical value (flame photometry)(9).
^bThe band head analyses by (7) and (8) lead to negative values of $w_e x_e$ (≈ -0.5).
^cQ, R, S heads; possibly quintet system.
^dStrong 0-0 sequence, multiple heads.
^eMultiple heads.
^f|A| \approx 41.
^gDifferent values for $w_e x_e$ suggested by (3) and (6).
 (1) See ref. (1) of MnBr.
 (2) Miescher, Müller, HPA 15, 319 (1942).
 (3) See ref. (2) of MnBr.
 (4) See ref. (3) of MnBr.
 (5) See ref. (4) of MnBr.
 (6) See ref. (5) of MnBr.
 (7) Hayes, Nevin, NC(Suppl.) 2, 734 (1955).
 (8) See ref. (8) of MnBr.
 (9) See ref. (9) of MnBr.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{55}\text{Mn}^{19}\text{F}$											
$\mu = 14.1166531$ $D_0^0 = 4.35 \text{ eV}^a$ Emission bands in the visible and near infrared: $\nu_e = 20298.2$; $w'_e = 637.1$, $w'_e x'_e = 1.9$; $w''_e = 649.1$, $w''_e x''_e = 1.5$; $\nu_e = 14527.7$; $w'_e = 595.4$, $w'_e x'_e = 3.15$; $w''_e = 645.4$, $w''_e x''_e = 3.2$;								b	R 20292.1	H^Q	(6)*
								c	R 20023.3 19971.6	H^R H^Q	(6)*
								d	R 14502.7	H^{QR}	(5)*
								e	ν_R 12179.6 12153.6	H^Q H^P	(4)*
B ($^7\Sigma$)	41231.5	637.2	H 4.46					B \leftarrow X,	V 41240.3	H	(1)*
A ($^7\Pi$)	28465.0 ^f	673 ^g	H 4					A \leftrightarrow X,	ν_R 28491.9 ^h	H	(1)(2)(3)*
X ($^7\Sigma$)	0	618.8 ⁱ	H 3.01								(7)*
$^{55}\text{Mn}^1\text{H}$											
$\mu = 0.98966996$ $D_0^0 = (2.5) \text{ eV}$ Complex rotational structure from 22600 to 24000 (max. 23360 - 23920) cm^{-1} ; in emission. Open but strongly perturbed rotational structure in the region 21270 - 22580 cm^{-1} ; in emission and absorption. Probably quintet transition. Extremely complicated R shaded band with very dense structure centered around 20900 cm^{-1} ; in emission and absorption. Probably quintet system. Complex rotational structure from 11200 to 14500 cm^{-1} ; in emission.										OCT 1975	
										(7)*	
										(2)* (7)*	
										(12)	
										(1)(2)* (7)*	
										(12)	
										(7)*	
A $^7\Pi$ a	17597 ^b	[1623] ^c	(33)	6.425 ^{de}	0.187	[3.62] ^f	1.628	A \leftrightarrow X,	V 17666 ^c		(1)(2)* (3)*
X $^7\Sigma$ a	0	1548.0	Z 28.8	5.6841 ^d	0.1570 ^g	[3.039] ^h	1.7311				(4)(5)* (7)
										(8)(10)(14)	
$^{55}\text{Mn}^2\text{H}$											
$\mu = 1.94287387$ $D_0^0 = (2.6) \text{ eV}$ Complex rotational structure in the region 23250 - 23800 cm^{-1} ; in emission. Complex R shaded rotational structure with heads at 22355 and 22564 cm^{-1} ; in emission and absorption.										OCT 1975	
										(7)*	
										(7)* (12)	

MnF: ^aThermochemical value (mass-spectrom.)(8).
^bComplex bands; R, Q heads.
^cTwo sequences of single heads, interpreted as R and Q heads.
^dFour heads.
^eSingle sequence of bands having apparently both Q and P (or R) heads.
^f $|A| \approx 25$.
^gAverage of (3) and (7).
^hStrongest head of F_4 component.
ⁱFrom B-X system.

(1) Rochester, Olsson, ZP 114, 495 (1939).
(2) Bacher, Miescher, HPA 20, 245 (1947).
(3) See ref. (3) of MnBr.
(4) See ref. (7) of MnCl.
(5) See ref. (6) of MnBr.
(6) See ref. (8) of MnBr.
(7) Rao, Reddy, Rao, PPS 72, 741 (1962).
(8) Kent, Ehlert, Margrave, JACS 86, 5090 (1964).

Mn¹H, Mn²H:

^aFor an ab initio calculation of these two states see (11).
^b $A = 40.6$ [see (14)].
^cFrom approximate origins for the F_4 component.
^dApproximate ("effective") constants. Improved ("true") constants for Mn¹H ($v=0$) together with spin-orbit, spin-spin, spin-rotation interaction and l -uncoupling constants in (14). See also (9) (13).
^ePerturbations.
^f $D_1 = 3.64 \times 10^{-4}$; $H_0 = 8.2 \times 10^{-9}$, $H_1 = 7.4 \times 10^{-9}$.
^g $\chi_e = -0.0019$.
^h $D_1 = 3.053 \times 10^{-4}$, $D_2 = 3.08 \times 10^{-4}$;
 $H_0 = 9.3 \times 10^{-9}$, $H_1 = 9.79 \times 10^{-9}$, $H_2 = 10.2 \times 10^{-9}$.
 H_v values in (13) differ by an order of magnitude.

(continued p.409)

Mn¹H, Mn²H (continued):

ⁱFrom the values for Mn¹H.

^jH₀ = 1.2 x 10⁻⁹.

^k*y*_e = -0.002₀.

^lD₁ = 8.22 x 10⁻⁵, D₂ = 8.36 x 10⁻⁵;

H₀ = 1.4₁ x 10⁻⁹, H₁ = 2.1₇ x 10⁻⁹, H₂ = 2.9₃ x 10⁻⁹.

(1) Heimer, Naturw. 24, 521 (1936).

(2) Pearse, Gaydon, PPS 50, 201 (1938).

(3) Nevin, PRIA A 48, 1 (1942).

(4) Nevin, PRIA A 50, 123 (1945).

(5) Nevin, Doyle, PRIA A 52, 35 (1948).

(6) Nevin, Conway, Cranley, PPS A 65, 115 (1952).

(7) Nevin, Stephens, PRIA A 55, 109 (1953).

(8) Hayes, McCarvill, Nevin, PPS A 70, 904 (1957).

(9) Kovács, PRIA A 60, 15 (1959).

(10) Kovács, Scari, APH 2, 423 (1959).

(11) Bagus, Schaeffer, JCP 58, 1844 (1973).

(12) Smith, PRS A 332, 113 (1973).

(13) Pacher, APH 35, 73 (1974).

(14) Kovács, Pacher, JP B 8, 796 (1974).

MnI: ^aThermochemical value (flame photometry)(3).

^bComplex system, incomplete analysis.

(1) Bacher, Miescher, HPA 20, 245 (1947).

(2) Bacher, HPA 21, 379 (1948).

(3) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

MnO: ^aThermochemical value (mass-spectrom.)(Burns, quoted in (9)(10)). Flame photometric values are approximately 4.1 eV (2)(5).

^bSeemingly continuous absorption, strongest in the region 38800-39100 cm⁻¹; some indication of band heads. It is not certain that this system is due to MnO.

MnO (continued):

^c*w y*_e = +0.06. Heads having v'=0 are ill defined.

^dPartial rotational analysis of the 1-0 band (13); spin-spin interaction constants λ' ≈ 0, λ'' = +0.66 cm⁻¹. Hyperfine broadening of all rotational lines; many bands are highly perturbed (12).

^eMatrix studies at 4 K (11) support the view that the lower state of A-X is the ground state.

(1) Sen Gupta, ZP 21, 471 (1934).

(2) Huldt, Lagerqvist, AF 3, 525 (1952).

(3) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(4) Das Sarma, ZP 157, 98 (1959).

(5) Padley, Sugden, TFS 55, 2054 (1959).

(6) Callear, Norrish, PRS A 259, 304 (1960).

(7) Joshi, SA 18, 625 (1962).

(8) Garrett, Lee, Kay, JCP 45, 2698 (1966).

(9) Cheetham, Barrow, AdHTC 1, 7 (1967).

(10) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).

(11) Thompson, Easley, Knight, JPC 77, 49 (1973).

(12) J.G. Kay, private communication (1974).

(13) Pinchemel, Schamps, CJP 53, 431 (1975).

MnS: ^aThermochemical value (mass-spectrom.)(1)(2)(3).

^bThermal emission, attributed to MnS.

(1) Colin, Goldfinger, Jeunehomme, Nature 194, 282 (1962).

(2) Wiedemeyer, Gilles, JCP 42, 2765 (1965).

(3) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).

(4) Monjazeb, Mohan, SpL 6, 143 (1973).

(5) Biron, Boulet, Ruamps, CR B 278, 835 (1974).

Mo₂: (1) Becker, Schürgers, ZN 26 a, 2072 (1971).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
(98)Mo ¹⁹ F		($\mu = 15.9109144$)	$D_0^0 = 4.78 \text{ eV}^a$							SEP 1976
(98)Mo ¹⁴ N ?		($\mu = 12.2508739_8$)	14 R shaded emission bands in the region $15840 - 16690 \text{ cm}^{-1}$, most of them previously be- lieved to be due to MoO (1), have been attributed (3) to a nitride, Mo _x N, of molybdenum on the basis of observed ¹⁴ N/ ¹⁵ N isotope shifts.							MAR 1975 (1)(3)
(98)Mo ¹⁶ O		($\mu = 13.7487642_2$)	$D_0^0 = 5.0 \text{ eV}^a$ Emission bands at $15358, 15511 \text{ cm}^{-1}$ (open structure), 11631 cm^{-1} (V), $11549, 11606, 11626 \text{ cm}^{-1}$ (R) are believed to be due to an oxide of molybdenum. Bands in the region $15930 - 16690 \text{ cm}^{-1}$, previously attributed to MoO, are due to Mo _x N.							MAR 1975 (1)(3)

MoF: ^aThermochemical value (mass-spectrom.)(1).

(1) Hildenbrand, JCP 65, 614 (1976).

MoN, MoO:

^aThermochemical value (mass-spectrom.)(2).

(1) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(2) De Maria, Burns, Drowart, Inghram, JCP 32, 1373 (1960).

(3) Howard, Conway, JCP 43, 3055 (1965).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}_2$		$\mu = 7.00153720$		$D_0^0 = 9.7594 \text{ eV}^a$			$\text{I.P.}(36_g) = 15.5808 \text{ eV}^b$ $(1\pi_u) = 16.6986 \text{ eV}^{bc}$ $(26_u) = 18.7507 \text{ eV}^b$ $(26_g) = 37.9 \text{ eV}^d$ $(1s_N) = 409.98 \text{ eV}^e$			FEB 1977 A

For a very detailed and critical review of the spectrum of molecular nitrogen and its ions see the recent publication by Lofthus and Krupenie (196). Atlas of the VUV absorption spectrum 1060-1520 Å and table of absorption lines (87). Tables of band head wavelengths (39)(48)(196). Photoionization and absorption cross sections (45)(57)(147). Potential functions (60)(68)(182)(196).

$x''(^1\Sigma_u^+)$	Several Rydberg series (excitation of $1s_N$) with limit (K edge) at 409.5 eV.	$x'' \leftarrow X,$	405.5 ₉ eV	} (114)(166) (173)(174)
$x'(^1\Pi_u)$	X-ray absorption ($3s \leftarrow 1s_N$).	$x' \leftrightarrow X,$	400.8 ₄ eV	
	X-ray absorption and emission ($1\pi_g \leftrightarrow 1s_N$), broad peak. ^f			
Photoionization and dissociative photoionization processes corresponding to various excited states of $N_2^+.$ ^g				(177)(194)
$v \quad ^1\Pi_g$	From high-energy electron impact spectroscopy.	$v \leftarrow X,$	253000	(180)
	Fragments of other progressions and unassigned bands, 198000 - 207000 cm^{-1} .			
u_5 (183640)	(2100) (15) } First two members of Codling's Rydberg series. ^h	$u_5 \leftarrow X,$	(183510)	} (76)(163)
u_4 (178565)	(2070) (15)	$u_4 \leftarrow X,$	(178420)	
	Hopfield's Rydberg series converging to $B \quad ^2\Sigma_u^+(v=0)$ of $N_2^+;$			
$\dots 26_u \quad 1\pi_u^4 \quad 36_g^2 \{ \begin{smallmatrix} ns6 \\ nd6 \end{smallmatrix} \}$	$v = 151233 - \left\{ \begin{smallmatrix} R/(m+0.141-0.199/m)^2, m = 3\dots 11 \text{ (apparent emission series)}^i \\ R/(m-0.070-0.041/m)^2, m = 3\dots 20 \text{ (absorption series)}^{jkl} \end{smallmatrix} \right.$			(1)(4)* (37)*
	Worley's ("third") Rydberg series joining on to o_3, o_4, o_5 and converging to $A \quad ^2\Pi_{u\frac{1}{2}}(v=0)$ of $N_2^+;$			
$\dots 26_u^2 \quad 1\pi_u^3 \quad 36_g^2 \quad ns6$	$v = 134721 - R/(n-1.06)^2, n = 3\dots 16.$ ^{mnop}			(8)(37)* (190)*
	Ogawa and Tanaka's Rydberg series joining on to o_4, o_5 and converging to $A \quad ^2\Pi_{u\frac{1}{2}}(v=0)$ of $N_2^+;$			
$\dots 26_u^2 \quad 1\pi_u^3 \quad 36_g^2 \quad ns6^q$	$v = 134644 - R/n^{*2}, n^* = 2.84, 3.85, 4.86, \dots, 14.91.$ ^{mnop}			(37)* (190)*
	Several dissociation continua in the region 100000 - 160000 cm^{-1} .			(105)(156)
	Several unidentified bands in the region 126100 - 131550 cm^{-1} .			(51)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
¹⁴ N ₂ (continued)										
s ^r	133355 133316	1885	H	(12)	Ogawa's	{ "new progression 4" o		s←X,	133119 H 133080 H	} (51)
r ^r	132878	1903	H	(15)		{ "new progression 3" os		r←X, R	132650 H	
q ^r	132136	1900	H	(18)		{ "new progression 2" os		q←X, t	131906 H	
p ^r	129136	1869	H	(10)		{ "new progression 1" os		p←X, R	128892 H	

- N₂: ^aFrom the predissociation in C ³Π_u assuming dissociation into ⁴S_{3/2} + ²D_{5/2}. The latest ab initio calculation of the ground state gives D_e = 8.58 eV (188).
^bFrom the Rydberg series.
^cAverage of the two limits corresponding to ²Π_{3/2} and ²Π_{1/2}.
^dFrom the data on N₂⁺.
^eFrom x→X of N₂⁺ and I.P.(N₂); the extrapolated K limit is 409.5 eV (114).
^fConfirmed by electron-energy-loss measurements (130). Preionization to X ²Σ_g⁺ and A ²Π_u of N₂⁺ observed by Auger electrons of 384.7 and 383.8 eV (119).
^gAbsorption cross sections 140000-500000 cm⁻¹ (163)(165).
^hThis series, of which only two members have been observed, probably converges to C ²Σ_u⁺ of N₂⁺. In u₄ v=1...13, in u₅ v=3...8 have been observed, but the vibrational numbering in both states is uncertain. Evidence of preionization.
ⁱLongward of the apparent emission "lines" are close-lying fairly sharp absorption "lines" (37). Both features belong to the same Fano shape produced by the interaction of the series of Rydberg levels with the continuum joining on to the A ²Π (or, less likely, X ²Σ) limit.

- ^jSimilar series with v'=1.
^kThe first three members at 138330, 144090, 146690 cm⁻¹ are very broad (presumably because of preionization), the higher members are sharper and shaded to the red. No rotational structure has been resolved. Preionization also observed by electron spectroscopy (162)(195).
^lOscillator strengths from absorption coefficients: f(m=3,4,...) = 0.0131, 0.0053, ... (126).
^mSimilar series for v'=1 [observed to n=45 (²Π_{1/2}) and n*=40.2 (²Π_{3/2})] and for v'=2...7 (190).
ⁿCorresponding series in ¹⁵N₂ (51).
^oPreionization observed in photoionization studies (58)(105)(161).
^pPreionization in absorption series having v'=1...4 was observed in active nitrogen using the photoionization technique (146).
^qInterpreted as ...nd₆ by (112).
^rThese designations should not be confused with the older designations of component states of b ¹Π_u and b' ¹Σ_u⁺.
^sPreionization also observed by electron spectroscopy (162)(195).
^tLine-like, not shaded.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}_2$ (continued)										
$o_5 \ ^1\Pi_u$	(127868)	(1935) ^a	(19)					$o_5 \leftarrow X$, R 127655	H^Q	(37)* (190)*
$o_5 ({}^3\Pi_u)$	127445	1925	H^Q	18.4				$o_5 \leftarrow X$, R 127227	H^Q	(37)* (190)*
Rydberg series converging to $X \ ^2\Sigma_g^+(v=0)$ of N_2^+ ; - Carroll and Yoshino's series joining on to c_4' , c_5' .										
$c_n \ ^1\Sigma_u^+ \dots 1\pi_u^4 3\sigma_g \text{np}^6$	^b									
- Ledbetter's series c_4 , c_5 , c_6 .										
- Worley and Jenkins' series joining on to c_3 , c_4 ; $v = 125666.8^c - R/(m + 0.3697 - 0.3459/m + 0.532/m^2 - 0.960/m^4)^2$, $m(\equiv n-1) = 2 \dots 31$.										
$o_4 \ ^1\Pi_u$	122419	[1824.1]	H			[1.7338] ^g	[4]	[1.1784]	$o_4 \leftarrow X$, R 122155.4	Z (37)(184)
$o_4 ({}^3\Pi_u)$	121263	1982	H	27.0					$o_4 \leftarrow X$, R 121071.1	H (37)
$c_5 \ ^1\Sigma_u^+$	(115876)	[2221.8]	Z	^h		[1.345] ⁱ			$c_5' \leftarrow X$, R 115849.8	Z (118)(144)*
$c_4 \ ^1\Pi_u$	115635.9	2220.3	Z	19.4		[1.926] ₁ ^j	0.01 ₅	[6.3] ^j	$c_4 \leftarrow a''$, 16725.1 ₂	Z (151)*
[A progression of six bands ($v''=1-6$) arises from $c_4(v'=0) \rightarrow a$, (11)]										
$z \ ^1\Delta_g$	(115435)	(1700)			1.761	0.0153		1.169	$z \rightarrow w$, V 43411.2 ^k	Z (25)
$y \ ^1\Pi_g$	114305.2 ^l	1906.43 ^l		37.51 ^l	1.739 ^{lm}	0.017 ^l	(5.8)	1.177	$y \rightarrow w$, V 42467.5 ⁿ	Z (26)* (175)
Kaplan II s.										
$y \rightarrow a'$, V 46426.7 ⁿ										
Kaplan I s.										
$k \ ^1\Pi_g$	(113808) ^o	[2182.32] ^l			1.959 ^l	0.031 ^l	(5.9)	1.109	$k \rightarrow w$, V 41932.4 ⁿ	Z (175)*
Carroll-Subbaram II s.										
$k \rightarrow a'$, V 45891.7 ⁿ										
Carroll-Subbaram I s.										
$x \ ^1\Sigma_g^-$	113438.0	1910.0	Z	20.7	1.750 ^p	0.0225	(6)	1.173	$x \rightarrow a'$, V 45472.8	Z (9)(23)*
5th pos. gr.										
$d' \begin{cases} ^1\Sigma_u^+ \\ ^1\Delta_u \end{cases}$ or	[112500]	Only $v'=0$ observed.								
									$d' \rightarrow a$, 42373	H (11)(12)(106)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
¹⁴ N ₂ (continued)										
$o_3 \ ^1\Pi_u$	105869 ^q	1987.4 ^q	16.3 ^q	1.7339 ^q	0.0088 ^q	(5.3)	1.1784	$o_3 \rightarrow a, \ v \ 36731$ $o_3 \leftarrow X, \ ^r R \ 105683$		(13)(15) (8)(184)
$H \ 3\phi_u$	(105720) ^s	924.21	z 12.29 ^t	1.0873	0.0191	[7.0] ^u	1.4881	$(H \rightarrow ?)^v \ 12407.2 \ H$ $H \rightarrow G, \ ^w v \ 17897.08^x Z$ Gaydon-Herman green s.		(17)(18) (10)(11)(19) (145)*

N₂: ^aVibrational intervals decrease irregularly; $v=0$ was shown [by electron spectroscopy (195)] to be preionized.
^bFor higher n values c_n and c_{n+1}' lie close together and interact strongly (l -uncoupling). Band structures for $n = 5 \dots 12$ have been discussed (144)(154)(186).
^cThe limit according to Yoshino [see (196)] lies at 125667.5 cm^{-1} but is estimated (196) to have an uncertainty of 5 cm^{-1} .
^dSimilar series with $v'=1$.
^eCorresponding series in ¹⁵N₂ (51).
^fSee P on p. 413.
^gOnly $v=0$ [perturbed by $c_6'(v=1)$] is sharp; bands with $v'=1, 2, 3$ are diffuse owing to predissociation or preionization (levels with $v \geq 2$ are above the first ionization potential).
^h $\Delta G(3/2) = 2119.7$, see ⁱ.
ⁱStrong homogeneous perturbations with the higher vibrational levels ($v \geq 18$) of $b' \ ^1\Sigma_u^+$ (144). The B_0 value is an effective value at low J ; $B_{\text{eff}}(v=1,2) = 1.28_5, 1.17_3$. In addition, there are heterogeneous interactions with the close-lying levels of $c_4 \ ^1\Pi_u$. For deperturbed constants see (152)(152a).
^jConstants for Π^- (151); $B_0(\Pi^+) = 1.906$. α_e from (144).
^kRe-evaluated from the origin of the 0-2 band. (25) gives 43667.0 which was undoubtedly calculated with the constants

of the a rather than of the w state.
^lStrong homogeneous interaction between $k \ ^1\Pi_g$ and $y \ ^1\Pi_g$. The constants given are the deperturbed values from (175) and refer to Π^- , the only component observed in $k \ ^1\Pi_g$.
^mPredissociation of the Π^+ component above $J=10$ of $v=0$. Λ -type doubling and predissociation discussed in (189).
ⁿNot deperturbed.
^oFrom the deperturbed $T_{00} = 113723.58$.
^pOnly $v'=0, 1, 2$ observed. Predissociation (weakening of emission) at $v'=2, J' \approx 15$ corresponding to the limit $^2D + ^2D$ (33); actual breaking-off occurs at $J'=25$. See also (189).
^qDeperturbed constants (184). Homogeneous interactions with levels ($v \geq 6$) of $b \ ^1\Pi_u$ and heterogeneous perturbations by $r \ ^1\Sigma_u^+$.
^rOscillator strengths (147).
^s $A_0 \dots A_3 = -12.073 \dots -12.094$ (145); see also (164).
^t $\omega_e v_e = -0.173$.
^u $D_{1,2,3}(10^{-6} \text{cm}^{-1}) = 4.5, 6.0, 5.0$ (145). See, however, (164).
^vFragment of near infrared spectrum, $\Delta G''(\frac{1}{2}) \approx 712$.
^wFranck-Condon factors and r -centroids (171).
^xFrom a more detailed theoretical treatment (164) derives $v_{00} = 17902.400$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}_2$ (continued)										
$c_4^+ 1\Sigma_u^+$	104519 ^a	2201.78 ^a	25.199 ^a	1.9612 ^a	0.0436 ^a		1.1080	$c_4^+ \rightarrow a$, V_R 35371.2 Z Gaydon-Herman b.		(12)(25)
								$c_4^+ \leftrightarrow X$, ^b R 104323.3 ^c		(55)(88)(104) (106)(118)
$c_3^+ 1\Pi_u$	104476 ^d	2192.20 ^d	14.70 ^d	1.9320 ^d	0.0395 ^d		1.1163	$c_3^+ \rightarrow a$, R_V 35187.0 (Z) $c_3^+ \leftrightarrow X$, ^e R 104138.2 ^f		(15) (104)(106)
$b^+ 1\Sigma_u^+$	104498 ^g	760.08 ^g	4.418 ^g	1.1549 ^{gh}	0.007387 ^g		1.4439	$b^+ \rightarrow a$, R ⁱ $b^+ \leftrightarrow X$, R 103673.8 ^j		(25) (22)(118)
								Birge-Hopfield b.		
D $3\Sigma_u^+$	[104746.6]	Only $v=0$ is observed		[1.961]		[20]	[1.108 ₀]	$D^k \rightarrow B$, V 44264.1 ^l 4th pos. gr.		(6)
b $1\Pi_u$	(101675)	[634.8] ^m		[1.448 ₃] ^{no}		[29] ^p	1.284 ₁ ^q	$b \rightarrow a$, R 31865.7 (Z) Gaydon-Herman b. $b \leftrightarrow X$, ^e R 100816.9		(9)(11)(25) (172) (104)(184)
$a'' 1\Sigma_g^+$	[100016.0]			[1.9133] ^r		[6.2] ^r	[1.1218]	$a'' \leftarrow X$, ^s 98840.30 ^r		(113)
$C^+ 3\Pi_u$	98351 ^t	791	33.5	[1.0496]	^u	[10.9] ^v	[1.514 ₆]	$C^+ \leftrightarrow B$, R 38255.5 ^w Goldstein-Kaplan b.		(44)* (191)* (198)*

N_2 : ^aDeperturbed constants (152)(152a); $w_e v_e = + 0.7874$. Strong perturbations produced by interaction with $b^+ 1\Sigma_u^+$; before these perturbations were recognized (106)(106a) the vibrational levels were attributed to independent states called p' , r' , k , s' , h , h' , h'' , h''' . The observed vibrational intervals (from band origins) and rotational constants for $v=0,1,2,3,\dots$ are:
 $\Delta G(v+\frac{1}{2}) = 2046.2, 2175.5, 2112.2, 2111.7 \dots$
 $B_v = 1.929, 1.711, 1.436, 1.594 \dots$

^bRadiative lifetime $\tau(v'=0) = 0.9 \text{ ns}$ (80)(99); oscillator strengths (98)(147).

^cObserved v_{00} , not deperturbed.

^dDeperturbed constants (152)(152a). Strong perturbations produced by interaction with $b^+ 1\Pi_u$; the observed vibrational intervals (from band heads) and rotational constants for $v=0,1,2,\dots$ are:
 $\Delta G(v+\frac{1}{2}) = 2401, 2146, 2103, 2042$;
 $B_v(\Pi^-) = 1.516, 1.755, 1.813$ [see (104)(152a)].

N₂ (continued):

^eOscillator strengths (98)(147).

^fQuoted from (196); not deperturbed. (106) gives 104139.

^gDeperturbed constants (152)(152a); $w_e y_e = + 0.1093$, ...
 $y_e = - 0.0000750$, ... Strong perturbations on account of interactions with c'_4 , c'_5 $^1\Sigma_u^+$. Before these perturbations were recognized (104)(106)(106a)(118) several of the vibrational levels were assumed to be independent states called b', g, f, r, s, t, u by (8). The observed vibrational intervals (from band origins) and rotational constants for $v=0, 1, 2, 3$, ... are:

$\Delta G(v+\frac{1}{2}) = 744.9, 732.9, 717.6, 777.7, \dots$ } highest obs'd
 $B_v = 1.1515, 1.15, 1.142, 1.152, \dots$ } level $v=28$.

Intensity perturb. in the electron energy loss sp. (108).

^hThe b'←X absorption bands show diffuseness indicating predissociation for $v'=20, 21, 22$ (118). Emission bands have only been observed to $v'=9$. For $v'=5$ and above $J'=12$ an intensity anomaly suggesting inverse predissociation has been observed in emission (56); it corresponds to the limit $^4S + ^2P$. Selective emission from $v'=0, 2, 7$ in discharges in Ar and Kr with traces of N₂ (94).

ⁱOnly the 7-0 band was observed at $v_0 = 40000.7$ (25).

^jObserved band origin, not deperturbed.

^kLifetime $\tau(v=0) = 14.1$ ns (159). Franck-Condon factors (110).

^lExtrapolated from $Q_2(3)$ of the 0-1 band.

^m $\Delta G(\frac{3}{2}, \frac{5}{2}, \dots) = 700.0, 711.9, 685.2, 1151.4, 646.2, \dots$
[(104), from band origins]. (152)(152a) give the deperturbed constants $w_e = 461.01$, $w_e x_e = - 132.257$, $w_e y_e = - 35.005$, $w_e z_e = + 5.822$, ...; see ⁿ.

ⁿ $B_v(v=1, 2, 3, \dots) = 1.4086, 1.3872, 1.3815, 1.4213, \dots$ (104); (152)(152a) give the deperturbed constants $B_e = 1.4601$,

$\alpha_e = 0.02624$, $y_e = - 0.00362$, ... Strong perturbations on account of interaction with the c_3 $^1\Pi_u$ and o_3 $^1\Pi_u$ Rydberg

states. Before these perturbations were recognized (104) (106) several of the vibr. levels were assumed to be independent electronic states called i, j, b, l, m, p, q (8). Intensity perturb. in the electron energy loss sp. (71)(108).

^oThe lines of absorption bands with $v'=0, 2, 3, 4$ are broadened on account of predissociation (especially $v'=3$); corresponding emission bands have not been observed. The state causing the predissociation is probably C' $^3\Pi_u$ (104); see, however, (137) who find that an additional diffuse level, very likely the still missing o_3 $^3\Pi_u(v=0)$ level at ~ 103000 cm^{-1} , is required to explain the broadening of $v'=3$.

^pEffective (perturbed) D_0 value.

^qFrom the deperturbed B_e (see ⁿ).

^rFrom Rydberg series having a" as lower state (151).

^sFirst thought to be observed as quadrupole absorption (90), later recognized as pressure-induced dipole transition represented by a broad diffuse absorption band at ~ 99005 cm^{-1} (113); note the large pressure shift of $+165$ cm^{-1} . The electron energy loss spectrum (81) shows a peak at 12.25 eV. Another $^1\Sigma_g^+$ state, non-Rydberg in character, is predicted to intersect a" not far from its minimum (129).

^t $A_0 = 2.10$, recalculated by (191) from the data of (44) who obtained 1.15; $A_1 = 2.73$, deperturbed value (191).

^u $B_1(\text{obs.}) = 1.2056$, $B_1(\text{depert.}) = 1.026$. Strong mixing of C'(v=1) with C(v=5). Deperturbed constants and RKR potential functions are given by (191) who have analyzed in detail the C'(v=1)←B(v=5) band for $^{14}\text{N}_2$, $^{14}\text{N}^{15}\text{N}$ and $^{15}\text{N}_2$. The perturbing level C(v=5) was recently observed by (198) in absorption from B(v=6).

^v $H_0 = 8.3 \times 10^{-10}$.

^w $v_{00} = 38296.75$ in (44) refers to the F₁ component.

State	T_e	m_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}_2$ (continued)										
E $3\Sigma_g^+$	(95858)	[2185]	H	[1.927 ₃]		[6.0]	[1.117 ₇]	E→B, V 36467.9 (Z) E→A, V 46019.7 ₂ Z Herman-Kaplan b. E←X, ^a	(107) (169)*	
C" $5\Pi_u$	(93500)	Arising from $^4S + ^2D$; according to (72) responsible for the main predissociation in C $3\Pi_u$.								
C $3\Pi_u$	89136.88 ^b	2047.17 ₈	Z 28.445 ₀ ^c	1.8247 ₃ ^d	0.01868 ^e		1.1486 ₉	C ^f →B, ^g V 29671.0 Z 2nd pos. gr. C←X, ^h R 88977.89 Z Tanaka b.	(1a)(29)(3)* (15a)* (53)* (21)(54) (67)*	
G $3\Delta_g$	(87900) ⁱ	[742.49]	Z 11.85 (H)	0.9280	0.0161	[5.0]	1.6107			
A' $5\Sigma_g^+$	(78800) ^j	(650) ^j	[For more recent results of an <u>ab initio</u> calculation see (199).]					(1.55) ^j		
w $1\Delta_u$	72097.4	1559.26 ^k	H 11.63	1.498 ^l	0.0166		1.268	w→a, ^m R 2747.29 Z McFarlane IR b. w←X, ^{hn} R 71698.4 ^o Z Tanaka b. a→a', ^m V 1212.28 Z McFarlane IR b. a ^s ↔X, ^t R 68951.20 Z Lyman-Birge-Hopfield b. a'↔X, ^w R 67739.31 Z Ogawa-Tanaka-Wilkinson-Mulliken b.	(84) (54)(155) (62)(83) (64)* (121) (30)* (65)* (103)(183) (155)	
a $1\Pi_g$	69283.06	1694.20 ₈	Z 13.949 ₁ ^p	1.6169 ^q	0.01793 ^r	(5.89)	1.2203			
a' $1\Sigma_u^-$	68152.66	1530.25 ₄	Z 12.0747 ^u	1.4799	0.01657 ^v	(5.55)	1.2755			

N_2 : ^aResonance-like electron impact excitation function centered at 12.2 eV with a half-width of 0.4 eV (143). Lifetime of $b_A = 39.2$ (2a). | the E state 190 μs (132).

^c $w_e v_e = + 2.0383_3$, $w_e z_e = - 0.5350$.

^dBreaking-off on account of predissociation (3) in $v'=1, 2, 3, 4$ above $N'=65, 55, 43, 28$, resp., yielding an accurate dis-

sociation limit at 97938 cm^{-1} ($^4S + ^2D$). A second prediss. in high-pressure discharges (when the first prediss. disappears) has been found in $v'=2$ and 3 above $N'=80$ and 67, respectively (7). According to (72) the first predissociation is caused by C" $5\Pi_u$, the second by C' $3\Pi_u$. Predissociation in $^{15}\text{N}_2$ (50). Intensity perturbations (1a)(3a)(3b).

N₂ (continued):

^e $= 0.00228(v+\frac{1}{2})^2 + 0.000733(v+\frac{1}{2})^3 - 0.00015(v+\frac{1}{2})^4$.

^f Lifetimes for $v=0,1,2$ vary between 35 and 41 ns (128)(136)(160)(178)(192). For f values of C-B see (47)(52).

^g The head of the 0-0 band produces laser oscillation; high resolution measurements of the laser lines (101), see also (91). An anomalous intensity alternation has been observed by (100), see also (93). C($v=5$) \leftarrow B($v=6$) band in absorption (198). ¹⁴N¹⁵N and ¹⁵N₂ isotope shifts (34). RKR Franck-Condon factors (73)(77), dependence on rotation (117). Integrated band intensities (38). Dependence of the electronic transition moment on r (139)(150); absolute transition probabilities (139).

^h RKR Franck-Condon factors (73)(75)(196).

ⁱ $A_0 = -0.21$, $A_1 = -0.25$. All constants for this state are from H \rightarrow G (145); for a more detailed theoretical treatment and somewhat different constants see (164).

^j From the predissociations in a and B (42); see also (27)(43). The dissociation energy of this state is estimated to be between 850 and 1100 cm⁻¹. According to (31) the ⁵ Σ_g^+ state plays an important role in the mechanism of the Lewis-Rayleigh afterglow of nitrogen.

^k Vibrational constants from the absorption spectrum (54), good agreement with band origin data for $k\rightarrow w$ (175).

^l Rotational constants from $y\rightarrow w$ (26).

^m Appears in stimulated emission.

ⁿ The $w\leftarrow X$ Tanaka bands appear diffuse even under high resolution (197) indicating that this is a pressure-induced transition which has apparently no measurable spontaneous

transition probability (187). Observed in solid N₂ by (92).

^o From $v_{00}(a-X) + v_{00}(w-a)$ (84). The value from the $w\leftarrow X$ absorption spectrum is 71740.3 (head) indicating a pressure shift of $\sim +40$ cm⁻¹; compare with $a'\leftarrow X$.

^p $w_e v_e = +0.007935$, $w_e z_e = +0.000291$, from (64); (196) give very slightly different numbers.

^q Small Λ -type doubling, $|q_0| = 0.00010$ (84). Breaking-off at low pressure above $v=6$, $J=13$ for both Λ components because of predissociation (16). The state causing the predissociation is ⁵ Σ_g^+ from ⁴S + ⁴S.

^r $r_{ge}^* = -0.0000293$.

^s The lifetime is about 100 μ s but depends strongly on v . Non-exponential decay because of radiative interactions with a' ¹ Σ_u^- and w ¹ Δ_u (148). See also (89)(140) who give f values.

^t This transition has both a magnetic dipole and an electric quadrupole component (28)(69), see also (140). Observed in absorption in solid N₂ by (92). RKR Franck-Condon factors (73)(75)(196). From intensity measurements and the Franck-Condon factors of (73) it is concluded by (82) that the electronic transition moment can be considered as constant for most bands of this system. Comparison with intensities in the electron energy loss spectrum (61).

^u $w_e v_e = +0.04129$, $w_e z_e = -0.000290$, from (65); (196) give very slightly different numbers.

^v $r_{ge}^* = +0.0000241$.

^w Franck-Condon factors (75)(196); $f_{00}(a'-X) = 8.4 \times 10^{-11}$, corresponding to a lifetime of 0.013 s (187).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
¹⁴ N ₂ (continued)										
B' $^3\Sigma_u^-$	66272.4 ₇	1516.88	Z 12.18 ₁ ^a	1.473 ₃ ^b	0.0166 ₆ ^c	(5.56)	1.278 ₄	B' → B, R 6545.5 (Z) "Y" bands, ^d		(32)(36) (182)
								B' ↔ X, ^e R 65852.35 Z Ogawa-Tanaka- Wilkinson b.		(30)* (35) (66)* (149) (155)
W $^3\Delta_u$	59808	1501.4	(Z) 11.6					W ↔ B, R, ^v 73 Wu-Benesch b.		(102)(124) (131)(157)
								W ← X, ^f R 59380 Saum-Benesch b.		(123)* (155)
B $^3\Pi_g$	59619.3 ₅ ^g	1733.39	Z 14.122 ^h	1.6374 ₅ ⁱ	0.0179 ₁ ^j	[5.9]	1.2126 ₀	B ^k ↔ A, ^l V 9552.0 ₃ Z 1st pos. gr.		(29)(196)
								B ← X, ^m R 59306.81 Z Wilkinson b.		(40)
A $^3\Sigma_u^+$	50203.6 ₃	1460.64	Z 13.87 ₂ ⁿ	1.4546 ^o	0.0180 ^p	[6.1 ₅]	1.2866	A ^q ↔ X, ^m R 49754.78 Z Vegard-Kaplan b.		(29)(70)(85)
X $^1\Sigma_g^+$	0	2358.57	Z 14.324 ^r	1.99824 ₁ ^s	0.017318 ^s	[5.76]	1.09768 ₅	Rot.-vibr. ^t and rot. sp. : - pressure induced - el. field induced Raman spectra ^u Mol. beam magn. reson. ^v		(14)(59)(63) (86)(135) (141)(181) (185) (20)(134) (167)

N₂: ^a $w_e y_e = + 0.0418_6$, $w_e z_e = - 0.000732$ (196).

^bSpin splitting constants ($v=5$): $\lambda = +0.66$, $\gamma = -0.0030$ (66).

^c $y_e = + 0.000009$ (196).

^dAlso referred to as "infrared afterglow bands".

^eRKR Franck-Condon factors (75)(196). Rotational intensity distribution (120).

^fFranck-Condon factors (123).

^g $A_e = 42.24$ (133).

N₂ (continued):

^h $w_e y_e = -0.0569$, $w_e z_e = +0.00361$ (196); slightly different constants are given by (74)(133).

ⁱPredissociation above $v=12, N=33$ (2)(153). The state causing the predissociation is probably A' $^5\Sigma_g^+$. Inverse predissociation A' $^5\Sigma_g^+ \rightarrow B$ $^3\Pi_g$ seems to be responsible for some of the phenomena in active nitrogen [see (142) and references quoted there]. The levels $v'=12, 11, 10$ are preferably excited in the Lewis-Rayleigh afterglow; for excitation of other levels in the afterglow see (193).

^j $y_e = -0.00007$ (196); slightly different constants in (133).

^kLifetime $\tau(v=0\dots 12) = 5.0 \mu s$ (176); see also (79). For B-A absorption f values (≈ 0.0025) see (41)(78)(97).

^lStimulated emission for some of the lines of the 4-2, 3-1, 2-0, 2-1, 1-0, 0-0, 0-1 bands has been observed (91). RKR Franck-Condon factors (73)(77), dependence on rotation (117). Dependence of the electronic transition moment on r (139) (150); absolute transition probabilities (111)(139).

^mFranck-Condon factors (75)(196). Rotational intensity distribution in the Vegard-Kaplan bands (122).

ⁿ $w_e y_e = +0.0103$, $w_e z_e = -0.00197$ (196); slightly different constants in (74)(133).

^oSpin splitting constants ($v=0$): $\lambda = -1.33$, $\gamma = -0.003$ (70); see also (133). The radio-frequency spectrum of this state was studied by the molecular beam magnetic resonance method (127)(158); magnetic hyperfine and electric quadrupole coupling constants.

^p $y_e = -0.00008$ (196).

^qLifetime 1.3 s for the F₂ levels, 2.5 s for the F₁ and F₃ levels (115)(116)(138); electronic transition moment, variation with r (96)(109)(115).

^r $w_e y_e = -0.00226$, $w_e z_e = -0.00024$ (196). (167) gives $\Delta G(\frac{1}{2}) = 2329.9168$ and similar data for $^{14}N^{15}N$ and $^{15}N_2$.

^sFrom B₀ and B₁ of (167) and using $\gamma_e = -0.000033$ from (196).

^tPredicted transition moments for quadrupole vibration spectrum (170). The quadrupole moment in the $v=0$ level is measured to be -1.4×10^{-26} e.s.u. cm² (46)(95).

^uRaman spectra of $^{14}N^{15}N$ and $^{15}N_2$ (167)(168).

^v $g_J(^{15}N_2) = 0.2593$, sign not determined (49). For magnetic resonance spectra of metastable N₂ in the A $^3\Sigma_u^+$ state see (127)(158).

(1) Hopfield, PR 35, 1133; 36, 789 (1930).

(1a) Coster, Brons, van der Ziel, ZP 84, 304 (1933).

(2) van der Ziel, Physica 1, 353 (1934).

(2a) Budó, ZP 26, 219 (1935).

(3) Büttnebender, Herzberg, AP(Leipzig) (5) 21, 577 (1935).

(3a) Gerö, ZP 26, 669 (1935).

(3b) Coster, Brons, ZP 27, 570 (1935).

(4) Takamine, Suga, Tanaka, Sci. Pap. IPCR (Tokyo) 34, 854 (1938).

(5) Worley, Jenkins, PR 54, 305 (1938).

(6) Gerö, Schmid, ZP 116, 598 (1940).

(7) Hori, Endo, PPMSJ 23, 834 (1941).

(8) Worley, PR 64, 207 (1943); 82, 863 (1953).

(9) Gaydon, PRS A 182, 286 (1944).

(10) Gaydon, PPS 56, 85 (1944).

(11) Herman, AP(Paris) (11) 20, 241 (1945).

(12) Gaydon, Herman, PPS 58, 292 (1946).

(13) Janin, Crozet, CR 223, 1114 (1946).

(14) Crawford, Welsh, Locke, PR 75, 1607 (1949).

(15) Janin, JRCNRS 3 (12), 156 (1950).

(15a) Herzberg, MOISPEC 1 (1950).

(16) Douglas, Herzberg, CJP 29, 294 (1951).

N₂ (continued):

- (17) Herman, CR 233, 738 (1951).
- (18) Carroll, Sayers, PPS A 66, 1138 (1953).
- (19) Grün, ZN 2 a, 1017 (1954).
- (20) Stoicheff, CJP 32, 630 (1954).
- (21) Tanaka, JOSA 45, 663 (1955).
- (22) Wilkinson, Houk, JCP 24, 528 (1956).
- (23) Lofthus, JCP 25, 494 (1956).
- (24) Hepner, Herman, AGEP 13, 242 (1957).
- (25) Lofthus, CJP 35, 216 (1957).
- (26) Lofthus, Mulliken, JCP 26, 1010 (1957).
- (27) Oldenberg, in "The Threshold of Space", p. 180, ed. Zelikoff (1957).
- (28) Wilkinson, Mulliken, ApJ 126, 10 (1957).
- (29) Dieke, Heath, Johns Hopkins Spectroscopic Report No. 17 (1959).
- (30) Ogawa, Tanaka, JCP 30, 1354 (1959); 32, 754 (1960).
- (31) Bayes, Kistiakowsky, JCP 32, 992 (1960).
- (32) Carroll, Rubalcava, PPS 76, 337 (1960).
- (33) Lofthus, Nature 186, 302 (1960).
- (34) Shvangiradze, Oganezov, Chikhladze, OS(Engl. Transl.) 8, 239 (1960).
- (35) Wilkinson, JCP 32, 1061 (1960).
- (36) Dieke, Heath, JCP 33, 432 (1960).
- (37) Ogawa, Tanaka, CJP 40, 1593 (1962).
- (38) Tyte, PPS 80, 1347, 1354 (1962).
- (39) Wallace, ApJ(Suppl.) 6, 445 (1962).
- (40) Wilkinson, JQSRT 2, 343 (1962).
- (41) Wurster, JCP 36, 2111 (1962).
- (42) Carroll, JCP 37, 805 (1962).
- (43) Mulliken, JCP 37, 809 (1962).
- (44) Carroll, PRS A 272, 270 (1963).
- (45) Huffman, Tanaka, Larrabee, JCP 39, 910 (1963).
- (46) Ketelaar, Rettschnick, MP 7, 191 (1963).
- (47) Nicholls, JATP 25, 218 (1963).
- (48) Pearse, Gaydon, IDSPEC (1963).
- (49) Chan, Baker, Ramsey, PR A 136, 1224 (1964).
- (50) Frackowiak, BAPS(MAP) 12, 361 (1964).
- (51) Ogawa, CJP 42, 1087 (1964).
- (52) Reis, JQSRT 4, 783 (1964).
- (53) Tyte, Nicholls, IAMS 2 (1964).
- (54) Tanaka, Ogawa, Jursa, JCP 40, 3690 (1964).
- (55) Tilford, Wilkinson, JMS 12, 231 (1964).
- (56) Tilford, Wilkinson, JMS 12, 347 (1964).
- (57) Cook, Metzger, JCP 41, 321 (1964).
- (58) Cook, Ogawa, CJP 43, 256 (1965).
- (59) Bosomworth, Gush, CJP 43, 751 (1965).
- (60) Gilmore, JQSRT 5, 369 (1965).
- (61) Lassetre, Meyer, Longmire, JCP 42, 807 (1965).
- (62) McFarlane, PR A 140, 1070 (1965).
- (63) Reddy, Cho, CJP 43, 2331 (1965).
- (64) Vanderslice, Tilford, Wilkinson, ApJ 141, 395 (1965).
- (65) Tilford, Wilkinson, Vanderslice, ApJ 141, 427 (1965).
- (66) Tilford, Vanderslice, Wilkinson, ApJ 141, 1226 (1965).
- (67) Tilford, Vanderslice, Wilkinson, ApJ 142, 1203 (1965).
- (68) Benesch, Vanderslice, Tilford, Wilkinson, ApJ 142, 1227 (1965).
- (69) Vanderslice, Wilkinson, Tilford, JCP 42, 2681 (1965).
- (70) Miller, JCP 43, 1695 (1965).
- (71) Meyer, Skerbele, Lassetre, JCP 43, 3769 (1965).
- (72) Carroll, Mulliken, JCP 43, 2170 (1965).
- (73) Zare, Larsson, Berg, JMS 15, 117 (1965).
- (74) Artym, OS(Engl. Transl.) Suppl. 2, 2 (1966).

N₂ (continued):

- (75) Benesch, Vanderslice, Tilford, Wilkinson, ApJ 143, 236 (1966).
(76) Codling, ApJ 143, 552 (1966).
(77) Benesch, Vanderslice, Tilford, Wilkinson, ApJ 144, 408 (1966).
(78) Dronov, Sobolev, Faizullov, OS(Engl.Transl.) 21, 301 (1966).
(79) Jeunehomme, JCP 45, 1805 (1966).
(80) Hesser, Dressler, JCP 45, 3149 (1966).
(81) Lassettre, Skerbele, Meyer, JCP 45, 3214 (1966).
(82) McEwan, Nicholls, Nature 209, 902 (1966).
(83) McFarlane, JQE 2, 229 (1966).
(84) McFarlane, PR 146, 37 (1966).
(85) Miller, JMS 19, 185 (1966).
(86) Shapiro, Gush, CJP 44, 949 (1966).
(87) Tilford, Wilkinson, Franklin, Naber, Benesch, Vanderslice, ApJ(Suppl.) 13, 31 (1966).
(88) Carroll, Yoshino, JCP 47, 3073 (1967).
(89) Ching, Cook, Becker, JQSRT 7, 323 (1967).
(90) Dressler, Lutz, PRL 19, 1219 (1967).
(91) Kasuya, Lide, AO 6, 69 (1967).
(92) Roncin, Damany, Romand, JMS 22, 154 (1967).
(93) Fishburne, Lazdinis, Seibert, JMS 23, 100 (1967).
(94) Tanaka, Nakamura, SL 16, 73 (1967).
(95) Buckingham, Disch, Dunmur, JACS 90, 3104 (1968).
(96) Chandraiah, Shepherd, CJP 46, 221 (1968).
(97) Cunio, Jansson, JQSRT 8, 1763 (1968).
(98) Lawrence, Mickey, Dressler, JCP 48, 1989 (1968).
(99) Hesser, JCP 48, 2518 (1968).
(100) Bleekrode, JCP 49, 951 (1968); Physica 44, 24 (1969).
(101) Parks, Rao, Javan, APL 13, 142 (1969).
(102) Wu, Benesch, PR 172, 31 (1968).
(103) Campbell, Thrush, TFS 65, 32 (1969).
(104) Carroll, Collins, CJP 47, 563 (1969).
(105) Comes, Weber, ZN 24 a, 1941 (1969).
(106) Dressler, CJP 47, 547 (1969).
(106a) Lefebvre-Brion, CJP 47, 541 (1969).
(107) Freund, JCP 50, 3734 (1969).
(108) Geiger, Schröder, JCP 50, 7 (1969).
(109) Broadfoot, Maran, JCP 51, 678 (1969).
(110) Hébert, Nicholls, JP B 2, 626 (1969).
(111) Kupriyanova, Kolesnikov, Sobolev, JQSRT 9, 1025 (1969).
(112) Lindholm, AF 40, 111 (1969).
(113) Lutz, JCP 51, 706 (1969).
(114) Nakamura, Sasanuma, Sato, Watanabe, Yamashita, Iguchi, Ejiri, Nakai, Yamaguchi, Sagawa, Nakai, Oshio, PR 178, 80 (1969).
(115) Shemansky, JCP 51, 689 (1969).
(116) Shemansky, Carleton, JCP 51, 682 (1969).
(117) Shumaker, JQSRT 9, 153 (1969).
(118) Carroll, Collins, Yoshino, JP B 3, 1127 (1970).
(119) Carlson, Moddeman, Pullen, Krause, CPL 5, 390 (1970).
(120) Kovács, OS(Engl. Transl.) 28, 239 (1970).
(121) Miller, JOSA 60, 171 (1970).
(122) Miller, PR A 1, 590 (1970).
(123) Saum, Benesch, PR A 2, 1655 (1970).
(124) Saum, Benesch, AO 2, 195 (1970).
(125) Vaidyan, Santaram, JCP 52, 3068 (1970).
(126) Cook, Ogawa, JCP 53, 1292 (1970).
(127) Freund, Miller, De Santis, Lurio, JCP 53, 2290 (1970).
(128) Johnson, Fowler, JCP 53, 65 (1970).

N₂ (continued):

- (129) Michels, JCP 53, 841 (1970).
- (130) Van der Wiel, El-Sherbini, Brion, CPL 7, 161 (1970).
- (131) Benesch, Saum, JP B 4, 732 (1971).
- (132) Borst, Zipf, PR A 3, 979 (1971).
- (133) Bullock, Hause, JMS 32, 519 (1971).
- (134) Butcher, Willets, Jones, PRS A 324, 231 (1971).
- (135) De Remigis, Welsh, Bruno, Taylor, CJP 49, 3201 (1971).
- (136) Imhof, Read, JP B 4, 1063 (1971).
- (137) Leoni, Dressler, ZAMP 22, 794 (1971).
- (138) Meyer, Klosterboer, Setser, JCP 55, 2084 (1971).
- (139) Shemansky, Broadfoot, JQSRT 11, 1385 (1971).
- (140) Pilling, Bass, Braun, JQSRT 11, 1593 (1971).
- (141) Sheng, Ewing, JCP 55, 5425 (1971).
- (142) Becker, Fink, Groth, Jud, Kley, DFS No. 53, 35 (1972).
- (143) Borst, Wells, Zipf, PR A 5, 648, 1744 (1972).
- (144) Carroll, Yoshino, JP B 5, 1614 (1972).
- (145) Carroll, Collins, Murnaghan, JP B 5, 1634 (1972).
- (146) Cook, McNeal, JCP 56, 1388 (1972).
- (147) Carter, JCP 56, 4195 (1972).
- (148) Freund, JCP 56, 4344 (1972).
- (149) Golde, Thrush, PRS A 330, 121 (1972).
- (150) Jain, JQSRT 12, 759 (1972).
- (151) Ledbetter, JMS 42, 100 (1972).
- (152) Leoni, Dressler, HPA 45, 959 (1972).
- (152a) Leoni, Dissertation (ETH Zürich, 1972).
- (153) Polak, Slovetskii, Sokolov, OS(Engl. Transl.) 32, 247 (1972).
- (154) Carroll, JCP 58, 3597 (1973).
- (155) Chutjian, Cartwright, Trajmar, PRL 30, 195 (1973).
- (156) Cook, Ogawa, Carlson, JGR 78, 1663 (1973).
- (157) Covey, Saum, Benesch, JOSA 63, 592 (1973).
- (158) De Santis, Lurio, Miller, Freund, JCP 58, 4625 (1973).
- (159) Kurzweg, Egbert, Burns, JCP 59, 2641 (1973).
- (160) Dotchin, Chupp, Pegg, JCP 59, 3960 (1973).
- (161) Carter, Berkowitz, JCP 59, 4573 (1973).
- (162) Hicks, Comer, Read, JP B 6, 165 (1973).
- (163) Lee, Carlson, Judge, Ogawa, JQSRT 13, 1023 (1973).
- (164) Veseth, MP 26, 101 (1973).
- (165) Watson, Lang, Stewart, JP B 6, L148 (1973).
- (166) Werme, Grennberg, Nordgren, Nordling, Siegbahn, Nature 242, 453 (1973).
- (167) Bendtsen, JRS 2, 133 (1974).
- (168) Butcher, Jones, JCS FT II 70, 560 (1974).
- (169) Carroll, Doheny, JMS 50, 257 (1974).
- (170) Cartwright, Dunning, JP B 7, 1776 (1974).
- (171) Mohamed, Khanna, IJPAP 12, 77 (1974).
- (172) Rajan, PRIA A 74, 17 (1974).
- (173) Vinogradov, Shlarbaum, Zimkina, OS(Engl. Transl.) 36, 383 (1974).
- (174) Vinogradov, Zimkina, Akimov, Shlarbaum, IANSF 38, 508 (1974). Engl. Transl. in BASPS 38, 69 (1974).
- (175) Carroll, Subbaram, CJP 53, 2198 (1975).
- (176) Chen, Anderson, PR A 12, 468 (1975).
- (177) Gardner, Samson, JCP 62, 1447 (1975).
- (178) Chen, Anderson, JCP 63, 1250 (1975).
- (179) Wong, Lee, Wellenstein, Bonham, JCP 63, 1538 (1975).
- (180) Lee, Wong, Bonham, JCP 63, 1643 (1975).
- (181) Buontempo, Cunsolo, Jacucci, Weiss, JCP 63, 2570 (1975).
- (182) Gartner, Thrush, PRS A 346, 103 (1975).
- (183) Golde, CPL 31, 348 (1975).
- (184) Yoshino, Tanaka, Carroll, Mitchell, JMS 54, 87 (1975).

N₂ (continued):

- (185) Courtois, Jouvé, JMS 55, 18 (1975).
- (186) Johns, Lepard, JMS 55, 374 (1975).
- (187) Tilford, Benesch, JCP 64, 3370 (1976).
- (188) Dunning, Cartwright, Hunt, Hay, Bobrowicz, JCP 64, 4755 (1976).
- (189) Mulliken, JMS 61, 92 (1976).
- (190) Yoshino, Ogawa, Tanaka, JMS 61, 403 (1976).
- (191) Ledbetter, Dressler, JMS 63, 370 (1976).
- (192) Osherovich, Gorshkov, OS(Engl. Transl.) 41, 92 (1976).
- (193) Ung, JCP 65, 2987 (1976).
- (194) Wight, Van der Wiel, Brion, JP B 2, 675 (1976).
- (195) Wilden, Hicks, Comer, JP B 2, 1959 (1976).
- (196) Lofthus, Krupenie, JPCRD 6, 113 (1977).
- (197) Tilford, Vanderslice, Tanaka, unpubl., quoted by (196).
- (198) Ledbetter, JCP 67, 3400 (1977).
- (199) Krauss, Neumann, MP 32, 101 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}_2^+$ **)		$\mu = 7.00140006$		$D_0^0 = 8.712_8 \text{ eV}^a$		$\text{I.P.} = 27.1 \text{ eV}^b$				MAR 1977 A
x		Several other much weaker X-ray emissions corresponding to higher levels of N_2^+ . K state of N_2 (removal of one K electron)						$x \rightarrow C, \quad 384.5 \text{ eV}^c$ $x \rightarrow B, \quad 391.33 \text{ eV}$ $x \rightarrow A,^d \quad 393.34 \text{ eV}$ $x \rightarrow X, \quad 394.40 \text{ eV}^e$	(47)(48)	
G $2\Sigma_g^+$ (195000)		Repulsive state corresponding to removal of a $2\sigma_g$ electron and dissociating into $\text{N}(^4\text{S}) + \text{N}^+(2s2p^3 \text{ } ^3\text{P})$, observed in photoelectron and photoion spectra with maximum at 39.8 and limit at 37.8_6 eV .							(58)	
C $2\Sigma_u^+$ 64608.1^f		2071.5^f	Z	9.2_9^g	[1.509 ₈]	hi	4.0	[1.262 ₈]	$C^j \rightarrow X, \text{ R } 64542.0$ Z 2nd neg. gr.	(9)(10)* (11)* (72)
D $2\Pi_{gi}$ 52318.2^k		907.7_1	Z	11.91^l	1.113	0.020	5	1.471	$D \rightarrow A, \text{ R } 42654.0$ Z Janin-d'Incan b.	(13)* (16)
(a $4\Sigma_u^+$) (25467)		(2398)	(14)		(2.071)	(0.014)			(a $\rightarrow X$) ^m (25563.26)	
B $2\Sigma_u^+$ 25461.4_6		2419.84	Z	23.18_9^n	b'	[2.07456] ^o p	0.024 ^q	[6.17]	$B^r \leftrightarrow X,^s \text{ } v_R 25566.04$ Z 1st neg. gr.	(1)* (1a)(6) (20)* (38) (73)
A $2\Pi_{ui}$ 9166.9_5^t		1903.7_0^u	Z	15.02	b'	1.7444^v p	0.0188_3^v	5.6^v	$A^w \rightarrow X,^x \text{ R } 9015.5_7$ Z Meinel b.	(8)(73)
X $2\Sigma_g^+$ 0		2207.00	Z	16.10^y	b'	1.93176^z p	0.01881	[6.10] ^{a'}		

N_2^+ : ^aFrom $D_0^0(\text{N}_2) + \text{I.P.}(\text{N}) - \text{I.P.}(\text{N}_2)$.

^bFrom the electron impact appearance potential of N_2^{++} (15) and I.P.(N_2). See also (39) and ref. given there.

^cVertical transition.

^dConsisting of a v progression ($v''=0\dots 5$).

^eObserved X-ray emission line leading to $X \text{ } 2\Sigma_g^+(v=0)$; the

value predicted from the K limit and I.P.(N_2) is 393.9 eV.

The X-ray line has a shoulder at 394.1_7 eV probably corresponding to $v''=1$.

^fDifferent constants are derived by (23) who assumes that the levels $v=0,1,2$ are perturbed and therefore does not include them in the evaluation; he gives $T_e = 64562.93 \text{ cm}^{-1}$.

N_2^+ (continued);

$\epsilon_{we}y_e = -0.43$. Vibrational numbering confirmed by ^{14}N - ^{15}N isotope shifts (7)(17)(24). Additional vibrational levels (to $v'=17$) observed by (49) in the photoelectron spectrum. $h\nu_B(v=1\dots6) = 1.5096, 1.5035, 1.4970, 1.4898, 1.4804, 1.4700$. The shape of the B_v curve is anomalous; meaningful equilibrium constants have not been determined. Spin doubling partially resolved for high N values (11).

ⁱIn a discharge through $He+N_2$ the $v'=3$ bands are strongly enhanced. It has been suggested (6) that this enhancement is due to inverse predissociation, i.e. $N(^4S) + N(^3P) \rightarrow N_2(C^2\Sigma_u^+)$; see also (11). Direct predissociation, i.e. the production of N^+ ions, has been observed mass-spectrometrically (35)(66); see also (30)(34). According to (35) the "metastable" ion $N_2^+(C^2\Sigma_u^+)$ has a lifetime of 0.8 μs before radiationless decomposition; see, however, (55) and ^j. The question which state causes the predissociation has been the subject of much discussion (54)(61)(62) following the discovery of a large isotope effect on this predissociation (43)(53)(55)(59). See also (36). Another predissociation limit at 26.70 eV above $N_2(X^1\Sigma_g^+, v=0)$ and corresponding to $^2D^0 + ^3P$ has been observed by (49).

^jRadiative lifetime of the non-predissociated levels $\tau(v \leq 2) = 0.09 \mu s$ (34).

$k_A = -16.5$.

$\epsilon_{we}y_e = +0.016$. Vibrational numbering confirmed by ^{14}N - ^{15}N isotope shifts (17).

^mThe identification of this quartet-doublet transition by (68) has been questioned by (70) who considers it as the 1st negative system of ^{14}N - $^{15}N^+$.

$\epsilon_{we}y_e = -0.5375$, $\epsilon_{we}z_e = -0.0495$; these constants, derived from ω_0 , ω_0x_0 , ... of (1a), represent the unperturbed vi-

brational levels only to $v=10$; for $v>10$ the ΔG curve shows a positive curvature. Levels observed up to $v=29$ (6).

^oSpin splitting constant $\gamma_0 = +0.0229$ (73); (67) give $\gamma'-\gamma'' = 0.015$. Rotational intensity distribution (67); see also (57).

^pPRKR potential functions (25), see also (22)(60).

^qValid only to $v=3$. Rotational perturbations by $A^2\Pi_u$ in $v = 1, 3, 5, 8, 9, 13$; see (1)(1a)(2)(3)(4)(38).

^rLifetime $\tau(v=0) = 60.5$ ns, see (42)(65) and earlier work quoted by them. Perturbed rotational levels (e.g. $v=1, N=13, 14$) have lifetimes up to 95 ns (52). (18) gives $f_{00} = 0.019$; the electronic f value at the wavelength of the 0-1 band is 0.034 (21).

^sObserved in absorption in flash discharges (28); laser-induced fluorescence (63). From intensity measurements (45) conclude that the electronic transition moment is nearly independent of r ; see, however, (18)(27)(32). Franck-Condon factors (31)(33)(72).

^t $A(v=2,3) = -74.62$, small J dependence (73).

^uFrom (16); (73) give $\Delta G(5/2) = 1813.327$. Levels observed in nitrogen ion beams to $v=30$ (46). Vibrational numbering confirmed by $^{15}N_2^+$ data (12).

^vFrom the rotational constants for $v=2,3$ (73); also Λ -type doubling constants. For higher but less accurate B_v values see (16). $\beta_e = +0.18 \times 10^{-6}$ (73).

^wLifetime varies from 13.9 μs for $v=1$ to 7.3 μs for $v=8$; see (40), who give references to earlier work, and (37)(46). Transition probabilities, f values (41); $f_{00} = 0.00168$.

^xThe bands were observed in the aurora (5) before they were discovered in the laboratory (8). Dependence of the (continued on p. 428)

N_2^+ (continued):

electronic transition moment on r (29)(41)(46)(69)(71).
 $y_{we}y_e = -0.040$. These constants (38) are only very slightly different from those implied by (6) who gives w_0 , w_0x_0 ...

(73) give $\Delta G(\frac{1}{2}) = 2174.728$.

^zFrom B_0 and B_1 of (73). Spin splitting constant $y^*(v=0,1) = +0.0083$ (73); see also (67).

^a $D_1 = 6.38 \times 10^{-6}$ (73); higher, less accurate D_v values in (38).

^bExperimental Franck-Condon factors for photoionization into these states from the ground state of N_2 (26)(33)(50); theoretical Franck-Condon factors (72)(74); see also (44)(51).

(1) Herzberg, AP(Leipzig) (4) 86, 189 (1928).

(1a) Coster, Brons, ZP 70, 492 (1931); 73, 747 (1932).

(2) Childs, PRS A 137, 641 (1932).

(3) Parker, PR 44, 90, 914 (1933).

(4) Brons, Physica 1, 739 (1934); PKNAW 38, 271 (1935).

(5) Meinel, ApJ 112, 562 (1950); 113, 583 (1951); 114, 431 (1951).

(6) Douglas, CJP 30, 302 (1952).

(7) Baer, Miescher, HPA 26, 91 (1953).

(8) Douglas, ApJ 117, 380 (1953).

(9) Tanaka, JCP 21, 1402 (1953).

(10) Wilkinson, CJP 34, 250 (1956).

(11) Carroll, CJP 37, 880 (1959).

(12) Liu, ApJ 129, 516 (1959).

(13) Tanaka, Namioka, Jursa, CJP 39, 1138 (1961).

(14) Wallace, ApJ(Suppl.) 6, 445 (1962).

(15) Dorman, Morrison, JCP 39, 1906 (1963).

(16) Janin, d'Incan, Stringat, Magnaval, RO 42, 120 (1963).

(17) Namioka, Yoshino, Tanaka, JCP 39, 2629 (1963).

(18) Nicholls, JATP 25, 218 (1963).

(19) Gilmore, JQSRT 5, 369 (1965).

(20) Tyte, Nicholls, IAMS 3 (1965).

(21) Wray, Connolly, JQSRT 5, 633 (1965).

(22) Joshi, JQSRT 6, 211 (1966).

(23) Joshi, PPS 87, 285 (1966).

(24) Joshi, PPS 87, 561 (1966).

(25) Singh, Rai, JMS 19, 424 (1966).

(26) Spohr, von Puttkamer, ZN 22 a, 705 (1967).

(27) Kiselyovskii, Shimanovich, OS(Engl. Transl.) 24, 266 (1968).

(28) Herzberg, CPAS 2, No. 15 (1968).

(29) Koppe, Koval, Grytsyna, Fogel, OS(Engl. Transl.) 24, 440 (1968).

(30) Fournier, Ozenne, Durup, JCP 53, 4095 (1970).

(31) Grandmontagne, Jorus, Vincent, JP(Paris) 31, 749 (1970).

(32) Brown, Landshoff, JQSRT 11, 1143 (1971).

(33) Comes, Speier, ZN 26 a, 1998 (1971).

(34) Fournier, van de Runstraat, Govers, Schopman, de Heer, Los, CPL 2, 426 (1971).

(35) Wankenne, Momigny, IJMSIP 7, 227 (1971).

(36) Fournier, Govers, van de Runstraat, Schopman, Los, JP(Paris) 33, 755 (1972).

(37) Gray, Roberts, Morack, JCP 57, 4190 (1972).

(38) Klynning, Pagès, PS 6, 195 (1972).

(39) Appell, Durup, Fehsenfeld, Fournier, JP B 6, 197 (1973).

(40) Peterson, Moseley, JCP 58, 172 (1973).

(41) Cartwright, JCP 58, 178 (1973).

(42) Dotchin, Chupp, Pegg, JCP 59, 3960 (1973).

N_2^+ (continued):

- (43) Govers, van de Runstraat, de Heer, JP B 6, L73 (1973).
- (44) Kosinov, Skovorodko, OS(Engl. Transl.) 35, 344 (1973).
- (45) Lee, Judge, JP B 6, L121 (1973).
- (46) Maier, Holland, JCP 59, 4501 (1973).
- (47) Werme, Grennberg, Nordgren, Nordling, Siegbahn, Nature 242, 453 (1973).
- (48) Werme, Grennberg, Nordgren, Nordling, Siegbahn, PRL 30, 523 (1973).
- (49) Åsbrink, Fridh, PS 2, 338 (1974).
- (50) Gardner, Samson, JCP 60, 3711 (1974).
- (51) Lee, Rabalais, JCP 61, 2747 (1974).
- (52) Dufayard, Negre, Nedelec, JCP 61, 3614 (1974).
- (53) Govers, Fehsenfeld, Albritton, Fournier, Fournier, CPL 26, 134 (1974).
- (54) Lorquet, Lorquet, CPL 26, 138 (1974).
- (55) van de Runstraat, de Heer, Govers, CP 3, 431 (1974).
- (56) Cartwright, Dunning, JP B 8, L100 (1975).
- (57) Désesquelles, Do Cao, Vaissade, JP(Paris) 36, 795 (1975).
- (58) Gardner, Samson, JCP 62, 1447 (1975).
- (59) Govers, van de Runstraat, de Heer, CP 2, 285 (1975).
- (60) Hajj, PL A 50, 427 (1975).
- (61) Tellinghuisen, Albritton, CPL 31, 91 (1975).
- (62) Roche, Lefebvre-Brion, CPL 32, 155 (1975).
- (63) Engelking, Smith, CPL 36, 21 (1975).
- (64) Thulstrup, Andersen, JP B 8, 965 (1975).
- (65) Smith, Read, Imhof, JP B 8, 2869 (1975).
- (66) Wankenne, Bolduc, Marmet, CJP 53, 770 (1975).
- (67) Bouchoux, Bacis, Goure, Lambert, JQSRT 16, 451 (1976).
- (68) d'Incan, Topouzkhanian, JCP 63, 2683 (1975); 64, 3494 (1976).
- (69) Wu, Shemansky, JCP 64, 1134 (1976).
- (70) Dressler, JCP 64, 3493 (1976).
- (71) Mandelbaum, Feldman, JCP 65, 672 (1976).
- (72) Lofthus, Krupenie, JPCRD 6, 113 (1977).
- (73) Colbourn, Douglas, JMS 65, 332 (1977).
- (74) Albritton, Schmeltekopf, Zare, "Diatomic Intensity Factors", Wiley, to be published.

**) Potential functions of the observed states (19). Predicted electronic states and potential functions (56)(64).
Table of band head wavelengths (14).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{14}\text{N}_2^{++}$										
		$\mu = 7.00126291$							MAY 1976 A	
		Following the early work of (3), (6) have recently given the results of detailed calculations of many low-lying singlet and triplet states. On the basis of this theoretical work the assignment of the observed transition to N_2^{++} seems very probable but not conclusive.								
D	$1\Sigma_u^+$ (62928)	(1910) ^a	[1.8644]	[7.1]	[1.1364]	D→X,	62903.1 ₈	2	(1)* (2)	
		A few intermediate states are suggested by Auger electron (4) and double charge transfer spectra (5).								
X	$1\Sigma_g^+$ ^b 0	(1960) ^a	[1.8801]	[6.9]	[1.1317]					
$^{14}\text{N}_2^-$										
		$\mu = 7.00167435$	$D_0^0 = 7.93 \text{ eV}^a$	$\text{I.P.} = -1.90_1 \text{ eV}^b$					MAY 1976 A	
		Theoretical calculations of N_2^- states (10).								
		Additional resonances in electron scattering at higher energies, several of them associated with the lowest N_2 Rydberg states which derive from $A^2\Pi_u$ of N_2^+ .							(6a)(7)(8)	
E	$2\Sigma_g^+$ (77150) ^c	(2180) ^c	(16) ^c		1.11 ₅ ^c				(4)	
		Two long progressions of shape resonances in electron scattering at 8.2-9.6 and 9.0-11.2 eV above $X^1\Sigma_g^+(v=0)$ of N_2 . They correspond to negative ion formation with subsequent decay to $A^3\Sigma_u^+$ and $B^3\Pi_g$, respectively, of neutral N_2 .							(5)(6)(7)	
X	$2\Pi_g$ 0 ^d	(1968) ^{ef}	(10) ^e		1.19 ₃ ^e	Vibr. Raman sp. ^f			(2)	
						ESR sp. ^g			(1)	

N_2^{++} : ^aEstimated from $(4B^3/D)^{\frac{1}{2}}$.

^bNot certain that this is the ground state. As for C_2 , a low-lying $^3\Pi_u$ state has been predicted (6).

(1) Carroll, CJP 36, 1585 (1958).

(2) Carroll, Hurley, JCP 35, 2247 (1961).

(3) Hurley, JMS 2, 18 (1962).

(4) Stalherm, Cleff, Hillig, Mehlhorn, ZN 24 a, 1728 (1969).

(5) Appell, Durup, Fehsenfeld, Fournier, JP B 6, 197 (1973).

(6) Thulstrup, Anderson, JP B 8, 965 (1975).

N_2^- : ^aFrom $D_0^0(N_2)$ and the electron affinities of N_2 and N, assuming for the latter -0.07 eV as given by (9).

^bFrom the energy difference (corrected for zero-point energy) of the potential minima given by (3); see ^e.

^cMolecular constants estimated by (4) from a short progression of three very sharp resonances in electron scattering at 11.48, 11.75, 12.02 eV above $X^1\Sigma_g^+(v=0)$ of N_2 . The parent is the $E^3\Sigma_g^+$ Rydberg state of N_2 , the grandparent $X^2\Sigma_g^+$ of N_2^+ .

^dThe minimum of the ground state potential function lies 1.92₅ eV above that of N_2 (3); see ^e.

^eGround state constants derived by (3) from a comparison of experimental with calculated cross sections for the vibrational excitation of N_2 by resonance scattering of electrons in the 2-4 eV region. The vibrational levels

N_2^- (continued):

have a considerable width owing to preionization, but the width parameter Γ decreases rapidly with increasing r from 0.57 eV at $r_e(N_2)$.

^f(2) observe $\Delta G(\frac{1}{2}) \approx 1840$ for N_2^- in potassium halide single crystals.

^gSpectrum of N_2^- in potassium halides, confirming the $^2\Pi$ nature of the ground state.

(1) Brailsford, Morton, Vannotti, JCP 50, 1051 (1969).

(2) Holzer, Murphy, Bernstein, JMS 32, 13 (1969).

(3) Birtwistle, Herzenberg, JP B 4, 53 (1971).

(4) Comer, Read, JP B 4, 1055 (1971).

(5) Snache, Schulz, PR A 6, 69 (1972).

(6) Mazeau, Greteau, Hall, Joyez, Reinhardt, JP B 6, 862 (1973).

(6a) Mazeau, Hall, Joyez, Landau, Reinhardt, JP B 6, 873 (1973).

(7) Schulz, RMP 45, 423 (1973).

(8) Golden, Burns, Sutcliffe, PR A 10, 2123 (1974).

(9) Hotop, Lineberger, JPCRD 4 (3), 539 (1975).

(10) Thulstrup, Andersen, JP B 8, 965 (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{23}\text{Na}_2$		$\mu = 11.4948852$ $D_0^0 = 0.720 \text{ eV}^a$ I.P. = 4.90 eV^b								JUN 1977 A	
		Diffuse bands of Na_2 vander Waals molecules close to the lines of the principal series of Na.								(5)(7)	
		Several fragments of other UV emission and absorption band systems. ^c								(4)(10)(13)	
E ($^1\Pi_u$)	35557.0	106.2	H 0.6 ₅					E \leftarrow X, R	35530.6 H	(15)(19)	
D ($^1\Pi_u$)	33486.8	111.3 ^d	H 0.4 ₈		e			D \leftrightarrow X, R	33462.9 H	(13)(15)(17)	
										(19)	
										(37)	
		Fragment observed in two-photon excited Na_2 fluorescence.									
C ($^1\Pi_u$)	(33000)	119.33 ^f	H 0.53		e			C \leftrightarrow X, R	29362 H	(12)(14)(17)	
B ($^1\Pi_u$)	29382	124.090	Z 0.6999 ^g		0.12527 ₇ ^h	0.000723 ₇ ⁱ	3.24 ₈ ^j	3.4228	B ^k \leftrightarrow X, ^l R	20302.49 ^m Z	(1)(6)(21)
A ($^1\Sigma_u^+$)	20320.02	117.323	Z 0.3576 ⁿ		0.11078 ₄ ^{op}	0.000548 ₈ ^q	3.88 ₂ ^r	3.6384	A ^s \leftrightarrow X, R	14659.80 Z	(30)
										(2)(8)(31)	
										(36)(40)	
a ($^3\Pi$)	14680.58	(145) ^t			(0.140) ^t						
X ($^1\Sigma_g^+$)	< 14680	159.124 ₅	Z 0.7254 ₇ ^u		0.154707 ^h	0.0008736 ^v	5.81 ₁ ^w	3.0788 ₇	Mol. beam magn. reson. ^x		
	0										

Na_2 : ^aFrom $D_e^0 = 5890 \pm 70 \text{ cm}^{-1}$ based on the RKR potential curve for the ground state (21)(30). The thermochemical value of (3), obtained by a molecular beam technique, is 0.73_2 eV .

^bFrom photoionization (20)(23). A similar value is obtained by extrapolation of the Rydberg series B,C,D,E (17)(19)(26).

^cMolecular absorption cross sections $27000 - 62500 \text{ cm}^{-1}$ (20).

^dVibrational constants from (15).

^e(17) report the following rotational constants for

D: $B_e = 0.1185$, $\alpha_e = 0.001$;

C: $B_e = 0.1281_5$, $\alpha_e = 0.0008_4$.

Considerably different constants, however, are quoted by Richards in (25):

D: $B_e = 0.1152$, $\alpha_e = 0.00110$;

C: $B_e = 0.1185$, $\alpha_e = 0.00096$.

^fVibrational constants from (14) (except T_e which has been recalculated). (17), without details, give $T_e = 29393$, $\omega_e = 117.3$, $\omega_e x_e = 0.5_5$, while Richards (25) quotes 29384.8 , 119.53 , and 0.782 , respectively.

^g $-0.00495(v+\frac{1}{2})^3 - 0.000153(v+\frac{1}{2})^4 + 7.01 \times 10^{-6}(v+\frac{1}{2})^5 - 1.804 \times 10^{-7}(v+\frac{1}{2})^6$; from the laser-induced fluorescence spectrum, including levels with $v' \leq 29$ (30). This state has a potential hump of $\sim 550 \text{ cm}^{-1}$ (0.069 eV); see (30), also (27). The non-appearance of levels with $v' > 26$ in the magnetic rota-

Na₂ (continued):

tion spectrum may be due to weak predissociation; see (11).

^hRKR potential functions (30).

$$i - 3.15_9 \times 10^{-5} (v + \frac{1}{2})^2 + 1.040 \times 10^{-6} (v + \frac{1}{2})^3 - 2.92_0 \times 10^{-8} (v + \frac{1}{2})^4.$$

The constants are for P and R lines, $B(R,P) - B(Q) = +0.000128$ (30).

$$j \beta_e = +4.75 \times 10^{-8}, \dots; H_e = -2.14_5 \times 10^{-11}, \text{ and higher order constants (30).}$$

^kRadiative lifetimes of 24 different levels (v', J') have been measured with an accuracy of $\sim 1\%$ by means of a delayed coincidence single-photon counting technique (34); the observed lifetimes [see also (22)(24)] vary from 7.0 to 7.5 ns and have been used to determine the electronic transition moment and its variation with r . The results are in good agreement with (28) and with the ab initio calculations of (39). See, however, (27)(29).

^lFranck-Condon factors, dependence on rotation (34).

^mThe band origin given here does not include $-B\Lambda^2$.

$$n + 5.167 \times 10^{-6} (v + \frac{1}{2})^3 + 9.277 \times 10^{-6} (v + \frac{1}{2})^4 - 1.456 \times 10^{-7} (v + \frac{1}{2})^5; \text{ from (40), see also (31). The observations extend to } v' = 44 \text{ (36)(40).}$$

^oRotational perturbations in $v=0$ and 1 are caused by levels belonging to the three components of the lower-lying $a^3\Pi$ state (31). Similar perturbations affect the higher vibrational levels and are responsible for the appearance of an A-X magnetic rotation spectrum (8)(9).

^pRKR potential function (40).

$$q + 1.625 \times 10^{-8} (v + \frac{1}{2})^2 + 3.165 \times 10^{-8} (v + \frac{1}{2})^3 - 9.205 \times 10^{-10} (v + \frac{1}{2})^4; \text{ from (40), see also (31).}$$

$$r H_e = +1.129 \times 10^{-12} \text{ (40), see also (31).}$$

^sRadiative lifetimes (35) are nearly constant for $1 \leq v \leq 25$, $\tau = 12.5 \pm 0.5$ ns, in very good agreement with theory (39).

^tConstants estimated from the perturbations in $A^1\Sigma_u^+$ (9), see ^o. (33) predict $T_e = 13500$, $\omega_e = 160$, $B_e = 0.154$.

$$u - 0.00109_5 (v + \frac{1}{2})^3 - 4.72 \times 10^{-5} (v + \frac{1}{2})^4 + 3.2_1 \times 10^{-7} (v + \frac{1}{2})^5 - 7.5_3 \times 10^{-9} (v + \frac{1}{2})^6; \text{ the analysis of the } B \rightarrow X \text{ system includes levels with } v'' \leq 46 \text{ (30).}$$

$$v - 3.14_6 \times 10^{-6} (v + \frac{1}{2})^2 - 2.40_0 \times 10^{-7} (v + \frac{1}{2})^3 + 4.8_4 \times 10^{-9} (v + \frac{1}{2})^4 - 8.7_3 \times 10^{-11} (v + \frac{1}{2})^5, \text{ from (30).}$$

$$w \beta_e = +3.59 \times 10^{-9}; H_e = +1.92 \times 10^{-12}, \text{ also higher order constants (30).}$$

^x $g_J = (+)0.0389_2 \mu_N$ (18). From the nuclear resonance spectrum (16) determined eqQ, but much improved hyperfine coupling constants eqQ and c [spin-rot. const., see also (38)] in the $v=0$, $J=28$ level have recently been obtained by (32) using a laser-fluorescence molecular-beam-resonance technique.

(1) Loomis, Wood, PR 32, 223 (1928).

(2) Fredrickson, PR 34, 207 (1929).

(3) Lewis, ZP 69, 786 (1931).

(4) Kimura, Uchida, Sci. Pap. IPCR (Tokyo) 18, 109 (1932).

(5) Kuhn, ZP 76, 782 (1932).

(6) Loomis, Nusbaum, PR 40, 380 (1932).

(7) Wurm, ZP 72, 736 (1932).

(8) Fredrickson, Stannard, PR 44, 632 (1933).

(9) Carroll, PR 52, 822 (1937).

(10) Yoshinaga, PPMJSJ 19, 847, 1073 (1937).

(11) King, Van Vleck, PR 55, 1165 (1939).

(12) Pearse, Sinha, Nature 160, 159 (1947).

(13) Sinha, PPS 59, 610 (1947).

(14) Sinha, PPS A 62, 124 (1949).

(continued on p. 435)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{23}\text{Na}_2^+$		$\mu = 11.4947480$	$D_0^0 = 0.96 \text{ eV}^a$						MAR 1977	
X $2\Sigma_g^+$	0	Theoretical calculations of excited state potential curves (1)(2)(3), oscillator strengths (4). (126) ^b						(0.117) ^b	(3.54) ^b	
$^{23}\text{Na}_2^-$		$\mu = 11.4950223$	$D_0^0 = (0.44) \text{ eV}^c$				I.P. = (0.27) eV^d		MAR 1977	
$^{23}\text{Na}^{40}\text{Ar}$		$\mu = 14.5940364$	$D_e^0 = 0.0052 \text{ eV}^a$						MAR 1977 A	
C $2\Sigma^+$		{ Bound state; continuous emission with maximum at $\sim 23580 \text{ cm}^{-1}$, shifted to the red by 2160 cm^{-1} from the forbidden Na 4s-3s line at 25740 cm^{-1} .						C \rightarrow X,	(5)	
B $2\Sigma^+$		{ Repulsive state except for a very small van der Waals minimum (2). Responsible for the far-blue-wing fluorescence spectrum of the Na D lines (16956 and 16973 cm^{-1}) in the presence of Ar gas.						B \rightarrow X,	(4)	
A 2Π		Attractive potential, $D_e = 550 \text{ cm}^{-1}$. ^b					3.17^b	A \rightarrow X,	(4)	
X $2\Sigma^+$	0	Unstable except for a small van der Waals minimum (2)(4)					4.8_1^a			
$^{23}\text{Na}^{79}\text{Br}$		$\mu = 17.803435_5$	$D_0^0 = 3.74 \text{ eV}^a$				I.P. = 8.3_1 eV^b		MAR 1977	
		The electron energy loss spectrum has peaks at 5.2, 7.1, 8.8, (20.0), 31.0 eV.							(13)	
		Continuous absorption above $\sim 30000 \text{ cm}^{-1}$ with maxima near 35500 and 40000 cm^{-1} . ^{cd}								
A		{ Diffuse absorption bands from 28800 to 22600 cm^{-1} ; in emission continua and diffuse bands from 31000 to 17000 cm^{-1} .						A \leftrightarrow X	(1)(2)(3)	

Na₂ (continued):

- (15) Chang, CJPS 2, 377 (1950).
- (16) Logan, Côté, Kusch, PR 86, 280 (1952).
- (17) Barrow, Travis, Wright, Nature 187, 141 (1960).
- (18) Brooks, Anderson, Ramsey, PRL 10, 441 (1963);
PR A 136, 62 (1964).
- (19) Morales, ARSEFQ A 52, 3 (1963).
- (20) Hudson, JCP 43, 1790 (1965).
- (21) Demtröder, McClintock, Zare, JCP 51, 5495 (1969).
- (22) McClintock, Demtröder, Zare, JCP 51, 5509 (1969).
- (23) Foster, Leckenby, Robbins, JP B 2, 478 (1969).
- (24) Baumgartner, Demtröder, Stock, ZP 232, 462 (1970).
- (25) DONNSPEC (1970).
- (26) Velasco, OPA 6 (2), 16 (1973).
- (27) Callender, Gersten, Leigh, Yang, PRL 32, 917 (1974);
PR A 14, 1672 (1976).
- (28) Hessel, Smith, Drullinger, PRL 33, 1251 (1974).
- (29) Williams, Rousseau, PRL 33, 1516 (1974).
- (30) Demtröder, Stock, JMS 55, 476 (1975).
- (31) Kusch, Hessel, JCP 63, 4087 (1975).
- (32) Rosner, Holt, Gaily, PRL 35, 785 (1975).
- (33) Bardsley, Junker, Norcross, CPL 37, 502 (1976).
- (34) Demtröder, Stetzenbach, Stock, Witt, JMS 61, 382 (1976).
- (35) Ducas, Littman, Zimmerman, Kleppner, JCP 65, 842 (1976).
- (36) Kaminsky, Hawkins, Kowalski, Schawlow, PRL 36, 671 (1976).
- (37) Woerdman, CPL 43, 279 (1976).
- (38) König, Weber, CPL 44, 293 (1976).
- (39) Stevens, Hessel, Bertoncini, Wahl, JCP 66, 1477 (1977).
- (40) Kaminsky, JCP 66, 4951 (1977).

Na₂⁺, Na₂⁻:

- ^aFrom $D_0^0(\text{Na}_2) + \text{I.P.}(\text{Na}) - \text{I.P.}(\text{Na}_2)$; theoretical values are $D_e^0 = 1.02$ eV (2) and 0.980 eV (3).
- ^bTheoretical calculations of (2); (3) predict $r_e = 3.3$ Å and $\omega_e = 109.2$, $\omega_e x_e = 0.21$ (4).
- ^cFrom $D_0^0(\text{Na}_2)$ and the electron affinities of Na₂ and Na.
- ^dEstimated on theoretical grounds (2).
- (1) Bottcher, Allison, Dalgarno, CPL 11, 307 (1971).
 - (2) See ref. (33) of Na₂.
 - (3) Cerjan, Docken, Dalgarno, CPL 38, 401 (1976).
 - (4) Kirby-Docken, Cerjan, Dalgarno, CPL 40, 205 (1976).

NaAr:

- ^aFrom atomic scattering data (1); see also (3).
- ^bMorse potential parameters from the analysis of the extreme-red-wing fluorescence spectrum of the sodium D lines (16956, 16973 cm⁻¹) in the presence of Ar gas (4); $\omega_e \approx 25$ cm⁻¹. See also (2).
- (1) Düren, Raabe, Schlier, ZP 214, 410 (1968).
 - (2) Baylis, JCP 51, 2665 (1969).
 - (3) Nikiforov, Shcherba, OS(Engl. Transl.) 32, 567 (1972).
 - (4) York, Scheps, Gallagher, JCP 63, 1052 (1975);
Scheps, Gallagher, JCP 65, 859 (1976).
 - (5) Tam, Moe, Bulos, Happer, OC 16, 376 (1976).

NaBr:

- ^aThermochemical value [(9)(16); flame photom.(10)].
- ^bOnset of a broad photoelectron peak with maximum at 8.80 eV, not corrected for thermal population of ground state levels (21). See also (20).
- ^cUV absorption cross sections (12). Absorption at higher energies produces fluorescence from Na(3p ²P), maximum efficiency at 50500 cm⁻¹ (19).
- (continued on p.437)

NaBr (cont'd), NaBr⁺:

^dThe absorption spectrum of NaBr trapped in inert gas matrices shows band structure at $\nu > 32300 \text{ cm}^{-1}$; under certain conditions as many as 16 peaks have been observed with spacings of approximately 453 and 523 cm^{-1} in Ar, 529 in Kr, and 472 in N₂ (17).

^eFrom the IR spectrum (8); $\omega_e = 298.4_9$ and $\omega_e x_e = 1.16$ have been calculated by (11) from the microwave results using Dunham's theory.

^f $\gamma_e = + 0.00000243$.

^g $\beta_e = - 0.0050 \times 10^{-7}$.

^h $\mu_{el}[D] = 9.091_8 + 0.0531(\nu + \frac{1}{2})$, $\nu \leq 2$ (14). (15), quoted in (18), gives eqQ values and their dependence on ν .

ⁱFrom $D_0^0(\text{NaBr}) + \text{I.P.}(\text{Na}) - \text{I.P.}(\text{NaBr})$. (21) give 0.49 eV using a corrected value of I.P.(NaBr).

^jFrom band maxima in the photoelectron spectrum (20)(21).

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Beutler, Josephy, ZP 53, 747 (1929).
- (3) Levi, Dissertation (Berlin, 1934).
- (4) Nierenberg, Ramsey, PR 72, 1075 (1947).
- (5) Logan, Coté, Kusch, PR 86, 280 (1952).
- (6) Coté, Kusch, PR 90, 103 (1953).
- (7) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (8) Rice, Klemperer, JCP 27, 573 (1957).
- (9) Brewer, Brackett, CRev 61, 425 (1961).
- (10) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (11) Rusk, Gordy, PR 127, 817 (1962).
- (12) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (13) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (14) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
- (15) Melendres, Thesis (U. of California, 1968).

NaCl, NaBr⁺ (continued):

- (16) JANAF (1971).
- (17) Oppenheimer, Berry, JCP 54, 5058 (1971).
- (18) Miller, Finney, Inman, AD 5, 1 (1973).
- (19) Earl, Herm, JCP 60, 4568 (1974).
- (20) Goodman, Allen, Cusachs, Schweitzer, JESRP 3, 289 (1974).
- (21) Potts, Williams, Price, PRS A 341, 147 (1974).

NaCl, NaCl⁺, NaCl⁻:

^aThermochemical value [(13)(21), flame photom.(10)(12)(14)].

^bAdiabatic potential from the onset of a broad photoelectron peak with maximum at 9.34 eV (23); not corrected for thermal population of ground state levels.

^cAlso observed in the electron energy loss spectrum (17) which has additional peaks at 7.1, 9.6, (20.5), 31.5 eV.

^dUV absorption cross sections (16).

^eFrom the IR spectrum (11). The Dunham relations applied to the microwave results of (15) give $\omega_e = 364.6_0$, $\omega_e x_e = 1.76$. In argon matrix $\Delta G(\frac{1}{2}) = 335$ (24).

^f $\gamma_e = + 0.0000051_4$.

^g $\beta_e = - 0.008_3 \times 10^{-7}$; $H_e = - 3.40 \times 10^{-14}$.

^hFor IR spectrum of matrix isolated sodium chloride see (24).

ⁱ $\mu_{el}[D] = 8.97141 + 0.05940(\nu + \frac{1}{2}) + 0.00025(\nu + \frac{1}{2})^2$, $\nu \leq 3$ (18) (20). For electric quadrupole coupling constants and their dependence on ν see (19)(20); earlier results by the magnetic resonance method.

^jFrom $D_0^0(\text{NaCl}) + \text{I.P.}(\text{Na}) - \text{I.P.}(\text{NaCl})$; (23) suggest 0.33 eV using a corrected value for I.P.(NaCl).

^kFrom band maxima in the photoelectron spectrum (22)(23).

^lFrom $D_0^0(\text{NaCl})$ and the electron affinities of NaCl and Cl.

^mEstimated electron affinity (25).

References on p. 439.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{23}\text{Na}^{133}\text{Cs}$		$\mu = 19.599483_0$ $D_e^0 = (0.42) \text{ eV}^a$ Fragment of another system overlapping C-X.								MAR 1977
C	(24270)	(62)	H					C \leftarrow X, (R) 24250	H	(1)* (2)
B	(18250)	(65)	H					B \leftarrow X, R 18233	H	(1)* (2)
X	$1\Sigma^+$ 0	(98)	H				(4.0) ^a	Mol. beam rf el. reson. ^b		
$^{23}\text{Na}^{19}\text{F}$		$\mu = 10.4021896$ $D_0^0 = (5.3_3) \text{ eV}^a$ The electron energy loss spectrum has peaks at 5.7, 7.7, (18.5), 32.5 eV. Continuous absorption above 41000 cm^{-1} . Fluctuation bands in absorption from 39350 to 36600 cm^{-1} .								MAR 1977
A								A \leftarrow X		(15) (1) (4)
X	$1\Sigma^+$ 0	536 ^{bc} (Z)	3.4 ^b	0.4369012 ₇	0.0045586 ₉ ^d	1.16 ₁	1.92594 ₇	Rot.-vibr. sp. ^c Rotation sp. Mol. beam rf electric ^e and magnetic reson.		(11)(14) (8)(10)(13) (10)(12) (2)(3)(5)

NaCs: ^aPotential data for the $1\Sigma^+$ ground state from total scattering cross-section measurements (3); see also (4).
(3) give also potential parameters for the $3\Sigma^+$ excited state ($D_e = 0.031 \text{ eV}$, $r_e = 6.2 \text{ \AA}$) which arises from the same atomic products $2S + 2S$.

^bFrom the measured Stark coefficient $\mu_0^2/B_0 = 1.81 \times 10^{-18} \text{ cm}^3$ and assuming $B_0 = 0.0631 \text{ cm}^{-1}$ (5) obtain $\mu_{eL}(v=0) = 4.7_5 \text{ D}$.

(1) Walter, Barratt, PRS A 119, 257 (1928).

(2) Weizel, Kulp, AP(Leipzig) 4, 971 (1930).

(3) Neumann, Pauly, PRL 20, 357 (1968); JCP 52, 2548 (1970).

NaCs (continued):

(4) Schlier, Vietzke, CPL 3, 250 (1969).

(5) Dagdigian, Wharton, JCP 57, 1487 (1972).

NaF: ^aValue recommended by (17) and based on the highest Na levels observed in chemiluminescent emission from the reaction $\text{Na}_2 + \text{F} \rightarrow \text{NaF} + \text{Na}^*$. It is in agreement with the flame-photometric value (5.2₅ eV) of (7), but substantially higher than the thermochemical value (4.9₃ eV) given by (6) or derived from the data in (16).

^bFrom the IR spectrum (11)(14).

NaF (continued):

^cFor IR frequencies in low-temperature rare gas matrices see (9).

$$d_{\text{Fe}}^{\text{d}} = + 0.00002335.$$

$\mu_{\text{eff}}^{\text{e}}[\text{D}] = 8.123_5 + 0.0644(v + \frac{1}{2}) + 0.0003_7(v + \frac{1}{2})^2$, $v \leq 2$ (10) (12); see also (8). Na quadrupole coupling constant, dependence on v (8)(10)(12); earlier, less accurate values by the magnetic resonance method (2)(3)(5).

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Zeiger, Bolef, PR 85, 788 (1952).
- (3) Logan, Coté, Kusch, PR 86, 280 (1952).
- (4) Barrow, Caunt, PRS A 219, 120 (1953).
- (5) Coté, Kusch, PR 90, 103 (1953).

NaF (continued):

- (6) Brewer, Brackett, CRev 61, 425 (1961).
- (7) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (8) Bauer, Lew, CJP 41, 1461 (1963); 42, 830 (1964).
- (9) Snelson, Pitzer, JPC 67, 882 (1963).
- (10) Hollowell, Hebert, Street, JCP 41, 3540 (1964).
- (11) Ritchie, Lew, CJP 42, 43 (1964).
- (12) Gräff, Werth, ZP 183, 223 (1965).
- (13) Veazey, Gordy, PR A 138, 1303 (1965).
- (14) Baikov, Vasilevskii, OS(Engl. Transl.) 22, 198 (1967).
- (15) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (16) JANAF (1971).
- (17) Ham, JCP 60, 1802 (1974).

NaCl, NaCl⁺, NaCl⁻ (continued):

- (1) See ref. (1) of NaF.
- (2) Levi, Dissertation (Berlin, 1934).
- (3) Nierenberg, Ramsey, PR 72, 1075 (1947).
- (4) See ref. (2) of NaF.
- (5) See ref. (3) of NaF.
- (6) Stitch, Honig, Townes, PR 86, 813 (1952).
- (7) See ref. (5) of NaF.
- (8) Ochs, Coté, Kusch, JCP 21, 459 (1953).
- (9) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (10) Gurvich, Veits, DPC 116, 639 (1957).
- (11) Rice, Klemperer, JCP 27, 573 (1957).
- (12) Gurvich, Veits, BASPS 22, 670 (1958).
- (13) See ref. (6) of NaF.

NaCl, NaCl⁺, NaCl⁻ (continued):

- (14) See ref. (7) of NaF.
- (15) Clouser, Gordy, PR A 134, 863 (1964).
- (16) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (17) See ref. (15) of NaF.
- (18) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
- (19) Cederberg, Miller, JCP 50, 3547 (1969).
- (20) de Leeuw, van Wachem, Dymanus, JCP 53, 981 (1970).
- (21) JANAF (1971).
- (22) Goodman, Allen, Cusachs, Schweitzer, JESRP 2, 289 (1974).
- (23) Potts, Williams, Price, PRS A 341, 147 (1974).
- (24) Ismail, Hauge, Margrave, JMS 54, 402 (1975).
- (25) Jordan, JCP 65, 1214 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{23}\text{Na}^1\text{H}$		$\mu = 0.96549966$ $D_0^0 = (1.88) \text{ eV}^a$							MAR 1977	
		Extensive theoretical calculations have been made of $X^1\Sigma^+$ (7)(9)(10)[see also (6)(8)] and of $A^1\Sigma^+$, $B^1\Pi$, $a^3\Sigma^+$, $b^3\Pi$, $c^3\Sigma^+$ (9); B , a , and c are predicted to be unstable. The calculations of (9) include transition moments, band strengths, line strengths, and the far-wing broadening of the sodium D lines; see also (14). Additional higher excited states have been computed by (11).								
b $^3\Pi$	(30940) ^b	(419) ^b	(50) ^b	(3.53) ^b	(0.85) ^b		(2.22) ^b	$A^f \leftrightarrow X$, R 22294.5 Z	(1)* (2)* (3)(4)	
A $^1\Sigma^+$	22719	310.6 ^c	Z	1.696 ^d		2.27 ^e	3.209			
X $^1\Sigma^+$	0	1172.2	Z 19.72 ^g	4.9012	0.1353 ^h	3.32 ^h	1.8874			
$^{23}\text{Na}^2\text{H}$		$\mu = 1.85186304$							MAR 1977	
A $^1\Sigma^+$		i		j		k		$A \leftarrow X$, R $v(7-0) = 24106.2$ Z	(3)	
X $^1\Sigma^+$	0	[826.1 ₀]	Z	2.5575	0.0520	0.915 ^l	1.8866			
$^{23}\text{Na}^4\text{He}$ $^{23}\text{Na}^4\text{He}^+$		$\mu = 3.4090714_3$							MAR 1977	
		Interaction potentials for $X^2\Sigma^+$, $A^2\Pi$, $B^2\Sigma^+$ have been calculated by (1)(2)(5)(6), for $X^1\Sigma^+$ by (2); see also (3). The coefficients of collision-induced absorption by Na-He in the region 0-300 cm^{-1} have been evaluated by (4).								
$^{23}\text{Na}^{127}\text{I}$		$\mu = 19.463754_1$ $D_0^0 = 3.00 \text{ eV}^a$ I.P. = 7.64 eV^b							MAR 1977 A	
		Peaks in the electron energy loss spectrum at 3.3, 5.7, 8.1, (20.0), 31.0 eV.							(15)	
		Dense, discrete rotational structure in absorption from 18500 to 33950 cm^{-1} (2)(8)(18), maximum of absorption at 30800. ^c At higher energies continuous absorption with maxima at ~ 38900								

$\text{Na}^1\text{H}, \text{Na}^2\text{H};$

^aTheoretical value as modified by (10); the computational results are $D_e^0 = 1.92$ (10) and 1.88 eV (9). Extrapolation of the ground state vibrational levels suggests 2.1 eV.

^bTheoretical predictions of (9) who feel, however, that the true potential of this state is considerably deeper than the calculated potential curve.

^cAnomalous potential curve [an RKR curve has been constructed by (5)]; $\Delta G(3/2 \dots 39/2) = 329.9, 337.2, 343.7, 349.6, 353.9, 357.4, 359.2, 360.3, 360.1, 359.5, 357.7, 354.3, 352.3, 348.4, 343.9, 340.0, 333.7, 330.0, 323.7$ [from band origins (4)].

^d $B_1 \dots B_7 = 1.823, 1.875, 1.908, 1.930, 1.938, 1.941, 1.936$ (4).

^e $H_e \approx 5.7 \times 10^{-8}$ (4); both D_v and H_v decrease with increasing v .

^fRadiative lifetimes $\tau(v'=3; J'=8) = 24.0$ ns, $\tau(4; 11) = 28.3$ ns, $\tau(5; 16) = 27.1$ ns (12); $\tau(8; 3) = 22.7$ ns (13).

^g $w_e v_e = +0.160, w_e z_e = -0.005$ (4).

^hRotational constants from (3), $\beta_e = -0.03 \times 10^{-4}$. (4) gives $B_e = 4.886, \alpha_e = 0.129, D_e \approx 3.15 \times 10^{-4}, H_e \approx 1.7 \times 10^{-8}$ but includes only levels with $v'' \geq 3$.

ⁱ $\Delta G(15/2 \dots 33/2) = 255.05, 256.92, 258.48, 259.39, 260.04, 260.22, 260.08, 259.61, 258.85, 257.6$ (from b. origins).

^j $B_7 \dots B_{17} = 1.010, 1.012, 1.012, 1.010, 1.007, 1.003, 0.998, 0.991, 0.984, 0.975, 0.95.$

^k $D_7 \dots D_{17} = 0.53 \times 10^{-4} \dots 0.44 \times 10^{-4}.$

^l $\beta_e = -0.009 \times 10^{-4}.$

(1) Hori, ZP 62, 352 (1930).

(2) Hori, ZP 71, 478 (1931).

(3) Olsson, ZP 93, 206 (1935).

(4) Pankhurst, PPS A 62, 191 (1949).

$\text{Na}^1\text{H}, \text{Na}^2\text{H}$ (continued):

(5) Jain, Sah, JCP 38, 1553 (1963).

(6) Varshni, Shukla, RMP 35, 130 (1963).

(7) Cade, Huo, JCP 47, 649 (1967).

(8) Cade, Bader, Henneker, Keaveny, JCP 50, 5313 (1969).

(9) Sachs, Hinze, Sabelli, JCP 62, 3367, 3377, 3384, 3389, 3393 (1975).

(10) Meyer, Rosmus, JCP 63, 2356 (1975).

(11) Numrich, Truhlar, JPC 72, 2745 (1975).

(12) Baltayan, Jourdan, Nedelec, PL A 58, 443 (1976).

(13) Dagdigian, JCP 64, 2609 (1976).

(14) Watson, Stewart, Dalgarno, MP 32, 1661 (1976).

$\text{NaHe}, \text{NaHe}^+;$

(1) Baylis, JCP 51, 2665 (1969).

(2) Krauss, Maldonado, Wahl, JCP 54, 4944 (1971).

(3) Bottcher, CPL 18, 457 (1973).

(4) Bottcher, Dalgarno, Wright, PR A 7, 1606 (1973).

(5) Pascale, Vandeplanque, JCP 60, 2278 (1974).

(6) Bottcher, Cravens, Dalgarno, PRS A 346, 157 (1975).

^aNaI: Dissociative photoionization of NaI (12). Thermochemical values (9) tend to be slightly higher, atomic fluorescence gives slightly lower values (neglecting, however, the thermal population of the ground state vibrational levels); for references see (12). Flame photometry suggests 3.13 eV (10).

^bFrom photoionization (12); in good agreement with the photoelectron spectrum (21).

^cIn inert gas matrices absorption bands from 25000 to 26000 cm^{-1} (19); the vibrational interval in Ar is ~ 166

(continued on p. 442)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{23}\text{Na}^{127}\text{I}$ (continued)										
X $1\Sigma^+$	0	and $46300\text{ cm}^{-1}(1)(2)^d$ Bands in emission from 24000 to $20000\text{ cm}^{-1}(2)$. 258^e (Z) (1.0_8) 0.1178056_1 0.0006477_7^f 0.973_4^g 2.71145_2					Rot.-vibr. sp. Rotation sp. Mol. beam rf electric ^h and magn. reson. ⁱ	(7) (6)(11) (16)(17) (3)(4)(5) (13)		
$^{23}\text{Na}^{127}\text{I}^+$										
A (2Σ)	9520^k	$D_0^0 = 0.50\text{ eV}^j$							MAR 1977	
X ($2\Pi_{1/2}$)	1770^k	Removal of an electron from the halogen 5p shell of Na^+I^- .								
X ($2\Pi_{3/2}$)	0^k									
$^{23}\text{Na}^{39}\text{K}$										
		$\mu = 14.4586992$	$D_0^0 = 0.62\text{ eV}^a$		$\text{I.P.} = 4.5\text{ eV}^b$				MAR 1977 A	
E	25228^c	95.8_5 H	0.94					E \leftarrow X, R 25214 H	(2)	
D (1Π)	20090.6	82.17 H	0.350^d					D \leftarrow X, R 20070.0 H	(1)(2)*	
C 1Π	16993.8	71.3_3 Z	1.236^e	0.0574_4	0.00007_8^f	32.1_1^g	4.50_5	C \leftarrow X, R 16967.2 Z	(1)(2)* (8)	
A ($1\Sigma^+$)	12139.7	79.85_2 H	0.0872^h	i				A \leftarrow X, R 12118.0 H	(1)	
X $1\Sigma^+$	0	124.134 Z	0.511^j	0.0905	0.000458_4^k	8.1_9^g	3.58_9	Mol. beam rf electric ^l and magn. reson. ^m	(5) (4)	
<u>Note:</u> It now appears that the ground state constants of (6) are unreliable; the uncertainty also affects the new results for the C state (8) [Arimondo, private comm.(1978)].										

Note: It now appears that the ground state constants of (6) are unreliable; the uncertainty also affects the new results for the C state (8) [Arimondo, private comm.(1978)].

NaI (continued), NaI^+ :

^dUV absorption cross sections (14).

^eFrom the IR spectrum (7). Application of the Dunham relations to the microwave results of (11) gives $\omega_e = 259.2_0$,

$\omega_e x_e = 0.96_4$.

^f $\gamma_e = + 0.00000143$.

^g $\beta_e = - 0.0005 \times 10^{-7}$.

^h $\mu_{el}[D] = 9.210_3 + 0.0507(v + \frac{1}{2})$, $v \leq 2$ (16). Electric quadrupole coupling constants, dependence on v (17); earlier

NaI, NaI⁺ (continued):

results by the magnetic resonance method (3)(4)(5).

ⁱ $g_J = (+)0.027 \mu_N$ (13).

^jFrom $D_0^0(\text{NaI}) + \text{I.P.}(\text{Na}) - \text{I.P.}(\text{NaI})$; (21) give 0.60 eV.

^kFrom the maxima in the photoelectron spectrum (20)(21).

- (1) Schmidt-Ott, ZP 62, 724 (1931).
- (2) Levi, Dissertation (Berlin, 1934).
- (3) Nierenberg, Ramsey, PR 72, 1075 (1947).
- (4) Logan, Coté, Kusch, PR 86, 280 (1952).
- (5) Côté, Kusch, PR 90, 103 (1953).
- (6) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (7) Rice, Klemperer, JCP 27, 573 (1957).
- (8) Berry, JCP 27, 1288 (1957).
- (9) Brewer, Brackett, CRev 61, 425 (1961).
- (10) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (11) Rusk, Gordy, PR 127, 817 (1962).
- (12) Berkowitz, Chupka, JCP 45, 1287 (1966).
- (13) Mehran, Brooks, Ramsey, PR 141, 93 (1966).
- (14) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (15) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (16) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).
- (17) Miller, Zorn, JCP 50, 3748 (1969).
- (18) Berg, Skewes, JCP 51, 5430 (1969).
- (19) Oppenheimer, Berry, JCP 54, 5058 (1971).
- (20) Goodman, Allen, Cusachs, Schweitzer, JESRP 3, 289 (1974).
- (21) Potts, Williams, Price, PRS A 341, 147 (1974).

NaK: (8) Allegrini, Moi, Arimondo, CPL 45, 245 (1977).

NaK: ^aExtrapolation of the vibrational levels in C ¹ Π assuming that this state has no potential maximum.

^bPhotoionization appearance potential (3).

^cRecalculated; (2) gives 25201 which must be erroneous.

^d $w_e y_e = -0.00814$.

^e $w_e y_e = +0.0088$, $w_e z_e = -0.000223$. All constants obtained from a study of the C state vibrational-rotational structure by laser excitation and collision-induced dissociation (8). Similar vibrational constants have been derived by (1) from absorption and magnetic rotation spectra; convergence limit at $18025 \pm 250 \text{ cm}^{-1}$ above X ¹ $\Sigma^+(v=0)$, corresponding to Na(²S) + K(4p ²P).

^f $y_e = -0.0000023$.

^gCentrifugal distortion constants as given by (8) and (6); there is no agreement with D_e values calculated from

$h_w y_e = -0.00389$. $| 4B_e^3/w_e^2$.

ⁱPerturbations (possibly by a ³ Π state) are very likely the cause for the appearance of a weak magnetic rotation sp..

$j - 7.9 \times 10^{-5}(v+\frac{1}{2})^3 - 2.47 \times 10^{-7}(v+\frac{1}{2})^4 - 2.50 \times 10^{-7}(v+\frac{1}{2})^5$ (6).

$k - 9.4 \times 10^{-7}(v+\frac{1}{2})^2 - 9.08 \times 10^{-8}(v+\frac{1}{2})^3$ (6).

^l $\mu_{el}(v=0) = 2.667 D$ [recalculated from $\mu_0^2/B_0 = 3.966 \times 10^{-19} \text{ cm}^3$ (5) with the new value for B_0]. Electric quadrupole coupling constants (5); see also (4).

^m $g_J = 0.0253 \mu_N$ (4). For an NMR experiment using optical pumping see (7).

- (1) Loomis, Arvin, PR 46, 286 (1934).
- (2) Sinha, PPS 60, 447 (1948).
- (3) Foster, Leckenby, Robbins, JP B 2, 478 (1969).
- (4) Brooks, Anderson, Ramsey, JCP 56, 5193 (1972).
- (5) Dagdigian, Wharton, JCP 57, 1487 (1972).
- (6) Toueg, Thesis (Columbia U., 1974), quoted by (8).
- (7) König, Weber, CPL 44, 293 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{23}\text{Na}^{(84)}\text{Kr}$										
C $^2\Sigma$		$(\mu = 18.045680_2)$				$D_e^0 = 0.0085 \text{ eV}^a$				MAR 1977
		{ Attractive potential; emission continuum with maximum at 23260 cm^{-1} , shifted to the red by 2480 cm^{-1} from the forbidden Na $4s-3s$ line at 25740 cm^{-1} .						C \rightarrow X,	(5)	
B $^2\Sigma$		{ Unstable except for a very small van der Waals minimum (2); respon- sible for the far-blue-wing fluorescence spectrum of the Na D lines (16956 and 16973 cm^{-1}) in a Kr atmosphere.						B \rightarrow X,	(4)	
A $^2\Pi$		Attractive potential; $D_e \approx 730 \text{ cm}^{-1}$. ^b						A \rightarrow X,	(4)	
X $^2\Sigma^+$	0	Repulsive except for a small van der Waals minimum (2)(4).						3.25^b 4.7_3^a		
$^{23}\text{Na}^{(20)}\text{Ne}$										
B $^2\Sigma$		$(\mu = 10.6932986)$				$D_e = (0.0050) \text{ eV}^a$	$(5.3)^a$			MAR 1977 A
A $^2\Pi$						$D_e = 0.014_9 \text{ eV}^a$	4.2_3^a			
X $^2\Sigma^+$	0					$D_e^0 = 0.0014 \text{ eV}^a$	4.8_2^a			
$^{23}\text{Na}^{16}\text{O}$										
A ($^2\Sigma$)	$(1500)^b$	$\mu = 9.4324071$				$D_0^0 = 2.6_0 \text{ eV}^a$				MAR 1977
X ($^2\Pi$)	0^b	$(548)^b$				$(0.470)^b$		$(1.95)^b$		
		$(526)^b$				$(0.425)^b$		$(2.05)^b$		
$^{23}\text{Na}^{16}\text{O}^+$										
		$D_0^0 = 0.8 \text{ eV}^c$								
$^{23}\text{Na}^{(85)}\text{Rb}$										
		$(\mu = 18.091514_0)$								MAR 1977
		A second system ($18400 - 18800 \text{ cm}^{-1}$) has not been analyzed.								(1)
A ($^1\Pi$)	16421.8	61.49	H	0.945				A \leftarrow X, (R) 16399.1	H	(2)
X ($^1\Sigma$)	0	106.64	H	0.455				Mol. beam el. deflection ^a		(3)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{23}\text{Na}(^{132})\text{Xe}$										
		$(\mu = 19.577567_2)$		$D_e^0 = 0.0124 \text{ eV}^a$						MAR 1977
C $^2\Sigma$		{ Attractive potential; continuous emission with maximum at 22690 cm^{-1} , shifted to the red by 3050 cm^{-1} from the forbidden Na 4s-3s line at 25740 cm^{-1} .						C \rightarrow X	(5)	
B $^2\Sigma$		{ Unstable except for a small van der Waals minimum (2); responsible for the far-blue-wing fluorescence spectrum of the Na D lines (16956 and 16973 cm^{-1}) in a Xe atmosphere.						B \rightarrow X,	(4)	
A $^2\Pi$		Attractive potential; $D_e = 1130 \text{ cm}^{-1}$. ^b						3.31^b	A \rightarrow X,	(4)
X $^2\Sigma^+$	0	Repulsive except for a small van der Waals minimum (2)(4).						4.91^a		

NaKr, NaXe:

^aFrom atomic scattering data (1); see also (2)(3).

^bMorse potential parameters from the analysis (4) of the extreme-red-wing fluorescence spectrum of the Na D lines in the presence of Kr or Xe gas; $\omega_e \approx 74$ or 83, respectively. See also (2).

- (1) Düren, Raabe, Schlier, ZP 214, 410 (1968).
- (2) Baylis, JCP 51, 2665 (1969).
- (3) Nikiforov, Shcherba, OS(Engl. Transl.) 32, 567 (1972).
- (4) York, Scheps, Gallagher, JCP 63, 1052 (1975);
Scheps, Gallagher, JCP 65, 859 (1976).
- (5) Tam, Moe, Bulos, Happer, OC 16, 376 (1976).

NaNe: ^aAll constants derived from high-resolution measurements of differential cross-sections for scattering of Na in the 2S ground and 2P excited states from Ne (3). There is serious disagreement with the pseudo-potential calculations of (1)(2).

NaNe (continued):

- (1) See ref. (2) of NaKr, NaXe.
- (2) Pascale, Vandeplanque, JCP 60, 2278 (1974).
- (3) Carter, Pritchard, Kaplan, Ducas, PRL 35, 1144 (1975).

NaO, NaO⁺:

^aThermochemical value [mass-spectrom.(2), calorim.(3)].

^bTheoretical results, average of two calculations (4)(6). The relative term values of the two states are in qualitative agreement with deductions made from a magnetic deflection analysis of the reactive scattering of Na + NO₂, see (1).

^cFrom a merging-beam study of the reaction CO⁺(Na,C)NaO⁺ (5). See also (4).

References on p. 447.

NaRb: See p. 447.

NaXe: See NaKr.

[illegible]

Nb₂: ^aAbsorption in Ar matrix at 14 K.

- (1) Green, Gruen, JCP 57, 4462 (1972).

NbN, NbO⁺:

^aConstants for the F₂ component. Large nuclear hyperfine structure in ³Δ₁ and ³Δ₃, b ≈ 0.196 cm⁻¹ (3). A smaller effect was also observed in the excited ³Φ state (3).

^bIR spectrum of Nb¹⁴N in Ar matrix at 14 K (2). Identity with the lower state of the gas phase sp. not certain.

- (1) Dunn, Rao, Nature 222, 266 (1969).
- (2) Green, Korfmacher, Gruen, JCP 58, 404 (1973).
- (3) Féménias, Athénour, Dunn, JCP 63, 2861 (1975); see also Féménias, Athénour, Stringat, CJP 52, 361 (1974); 53, 542, 2353(erratum) (1975).

NbO: ^aThermochemical value (mass-spectrom.) (6).

^bThe rotational analysis by (3) of seven bands in the G-X system assumed that they represent a ²Δ-²Δ transition. More recently, additional branches were found (7)(8) having very wide nuclear hyperfine structure [b ≈ 0.19 cm⁻¹ (12), as compared to 0.165 cm⁻¹ from the matrix ESR spectrum (11)]. The four branches of (3) probably represent the F₂ and F₃ components of the ⁴Σ⁻-⁴Σ⁻ transition. The rotational analysis by (4) appears to be in error.

NbO (continued):

^cOnly observed in a Ne matrix where the F state interacts with the nearby G ⁴Σ⁻ state.

^dAbsorption in rare gas matrices. Data are for Ne except for E←X which is only observed in Ar. So far, no satisfactory analysis was given for the complex systems of R shaded emission bands in the gas phase spectrum from 13300 to 18200 cm⁻¹ (1)(2)(5)*; see, however, (8)(12).

^eIn rare gas matrices.

- (1) Rao, IJP 24, 35 (1950).
- (2) Rao, Premaswarup, IJP 27, 399 (1953).
- (3) Uhler, AF 8, 265 (1954).
- (4) Rao, Nature 173, 1240 (1954); PNISI A 21, 188, 219 (1955).
- (5) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (6) Shchukarev, Semenov, Frantseva, ZNK 11, 233 (1966). Engl. transl. in RJIC 11, 129 (1966).
- (7) D. Richards, Thesis (Oxford, 1969).
- (8) Dunn, in "Molecular Spectroscopy: Modern Research" (ed. Rao and Mathews), p. 231. Academic Press (1972).
- (9) Singh, Shukla, JQSRT 12, 1249 (1972).
- (10) See ref. (2) of NbN.
- (11) Brom, Durham, Weltner, JCP 61, 970 (1974).
- (12) See ref. (3) of NbN.

NaO, NaO⁺: (1) Herm, Herschbach, JCP 52, 5783 (1970).

(2) Hildenbrand, Murad, JCP 53, 3403 (1970).

(3) O'Hare, JCP 56, 4513 (1972).

(4) O'Hare, Wahl, JCP 56, 4516 (1972).

(5) Rol, Entemann, Wendell, JCP 61, 2050 (1974).

(6) So, Richards, CPL 32, 227 (1975).

NaRb: ^aμ²/B = 6.6 x 10⁻¹⁹ cm³; assuming B = 0.0734 cm⁻¹ (3) derive an electric dipole moment of 3.1 D.

(1) Walter, Barratt, PRS A 119, 257 (1928).

(2) Kusch, PR 42, 218 (1936).

(3) Dagdigian, Wharton, JCP 57, 1487 (1972).

NBr: ^aEstimated from the highest ν' value observed in $b \rightarrow X$ emission from the reaction $N(^4S) + Br(^2P_{3/2}) \rightarrow NBr^* \rightarrow NBr + h\nu$ (2).
^bPotential functions (4).
^cFranck-Condon factors (5).
^dOnly levels with $N = J+1$, i.e. $F_1(N)$ corresponding in case "c" to the 0^+ component, have been observed at high resolution. For this reason, and since only B_3'' and B_7'' have been determined (assuming $\lambda \approx 8.7$, $\gamma \approx -0.7$) the values of B_e and α_e are not very precise.
^eIn argon and nitrogen matrices, $\Delta G(\frac{1}{2}) = 691$.
 (1) Elliott, PRS A 169, 469 (1939).
 (2) Milton, Dunford, Douglas, JCP 35, 1202 (1961).
 (3) Milligan, Jacox, JCP 40, 2461 (1964).
 (4) Singh, Rai, IJPAP 4, 102 (1966).
 (5) Itagi, Shamkuwar, Itagi, IJP 45, 385 (1971).

NC1: ^aSpin coupling constants $\lambda_0 = 1.776$, $\gamma_0 = -0.00715$.
^bIn argon and nitrogen matrices, $\Delta G(\frac{1}{2}) = 825$.
 (1) Milligan, JCP 35, 372 (1961).
 (2) See ref. (3) of NBr.
 (3) Colin, Jones, CJP 45, 301 (1967).

NdF: ^aThermochemical value (mass-spectrom.)(1).
 (1) Zmbov, Margrave, JCP 45, 3167 (1966).

NdO: ^aThermochemical value (mass-spectrom.)(4), recal. (5).
 (1) Piccardi, AANL (Ser. 6) 21, 584 (1935).
 (2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
 (3) Herrmann, Alkemade, "Chemical Analysis by Flame Photometry", Interscience (1963).
 (4) Ames, Walsh, White, JPC 71, 2707 (1967).
 (5) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

NdS: ^aThermochemical value (mass-spectrom.)(1), recal. (2).
 (1) See ref. (5) of NdO.
 (2) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

NdSe, NdTe:
^aThermochemical value (mass-spectrom.)(1).
 (1) See ref. (2) of NdS.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
(20)Ne ₂ (continued)											
a $3\Sigma_u^+$		Not observed in absorption from the ground state, but tentatively assigned as lower state of an absorption at 12270 cm^{-1} in Ne (200-1060 torr) excited by high-current short-duration electron bursts from a Febetron source (10); lifetime $\tau \approx 6.6_2 \text{ }\mu\text{s}$.									
x $1\Sigma_g^+$	0	[13.7] ^k H		[0.17] (0.06)			[3.1 ₅]				
(20)Ne ₂ ⁺											
		$D_e^0 = 1.30 \text{ eV}^a$								MAR 1977	
		Theoretical potential functions for the ground state and excited states arising from $1S + 2P_{\frac{3}{2}, \frac{1}{2}}$ (4).									
x $2\Sigma_u^+$	0	(510) ^b		(0.554) ^b			(1.75) ^b			Footnotes and references on p.453.	

Ne₂: ^aFrom $\Delta G''(\frac{1}{2})$ observed in the VUV absorption spectrum (4) and the binding energy of $v=1$ (6) as corrected by (7).
 (7) recommend $D_e^0 = 28.6 \text{ cm}^{-1}$ (0.0035₅ eV), a value derived from solid-state data (5a) and in fair agreement with the Ne-Ne scattering data of (2) and (5) [31.9 and 29.7 cm^{-1} , resp.] and the ab initio calculations of (3) and (8) [28.2 and 27.2 cm^{-1} , resp.]; see also (11) who give 30.2.
^bLowest observed level and interval $\Delta G(v+\frac{1}{2})$; the first observed band may not have $v'=0$.
^cIt is not certain that these two progressions belong to two separate electronic states.
^dAll bands are very diffuse.
^eIrregular intervals and intensities; tentative classification.
^fRotational structure partially resolved. | cation.
^gAlso weaker progression with $v''=1$.
^hDiffuse bands.

ⁱ $\Delta G(v+\frac{3}{2}) = 93$, $\Delta G(v+\frac{5}{2}) = 40$.
^jAttributed to $A \rightarrow X$ (4), possibly also contributions from
^kZero-point energy 12.3 cm^{-1} [see (7)]. | $a \rightarrow X$.
 (1) Tanaka, Jursa, LeBlanc, JOSA 48, 304 (1958).
 (2) Siska, Parson, Schafer, Lee, JCP 55, 5762 (1971).
 (3) Gordon, Kim, JCP 56, 3122 (1972).
 (4) Tanaka, Yoshino, JCP 57, 2964 (1972).
 (5) Farrar, Lee, Goldman, Klein, CPL 19, 359 (1973).
 (5a) Goldman, Klein, JLTTP 12, 101 (1973).
 (6) Tanaka, Yoshino, Freeman, JCP 59, 564, 5748(erratum)
 (7) Le Roy, Klein, McGee, MP 28, 587 (1974) | (1973).
 (8) Stevens, Wahl, Gardner, Karo, JCP 60, 2195 (1974).
 (9) Cohen, Schneider, JCP 61, 3230, 3240 (1974).
 (10) Oka, Rao, Redpath, Firestone, JCP 61, 4740 (1974).
 (11) Nain, Aziz, Jain, Saxena, JCP 65, 3242 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References	
								Design.	v_{00}		
(20)Ne⁴⁰Ar											
X $1\Sigma^+$	0	($\mu = 13.3257930_g$)		$D_e^0 = 0.0062$ eV ^a						MAR 1977	
		$[(20.9)]^b$		$D_0^0 = (0.0045)$ eV ^b			3.43 ^a		Translational sp. ^c	(1)	
(20)Ne⁴⁰Ar⁺											
A ₃ ($\frac{1}{2}$)	(46960) ^a	Five band groups [called A,B,C,D,E by (1)] with some vibrational structure which has, however, not been assigned.						A ₃ →X ₂	45380	(1)	
A ₂ ($\frac{3}{2}$)	(46180) ^a							A ₃ →X ₁	46960		
A ₁ ($\frac{1}{2}$)	(45920) ^a							A ₂ →X ₂	44590		
X ₂ ($\frac{1}{2}$)	(1585) ^a							A ₂ →X ₁	46180 ^b		
X ₁ ($\frac{1}{2}, \frac{3}{2}$)	0 ^a							A ₁ →X ₁	45920		
(20)Ne¹⁹F											
		($\mu = 9.7413757_g$)	No experimental results. Theoretical potential energy curves for X $2\Sigma^+$ and A 2Π (1).								MAR 1977 A
(20)Ne¹H											
		($\mu = 0.95945861$)	No spectra observed, all data are theoretical (5):								MAR 1977
C $2\Sigma^+$	(78170) ^a	(2737) ^b							(14.8)	(1.089)	
B 2Π	(70200) ^a	(2913)	(18.0)	(0.988)							
A $2\Sigma^+$	(70000) ^a	(2801)	(17.7)	(0.996)							
X $2\Sigma^+$	0 ^a	Repulsive st. with van der Waals minimum.									
(20)Ne¹H⁺											
				$D_0^0 = 2.08$ eV ^c						MAR 1977	
X $1\Sigma^+$		(2917) ^d	(18.0) ^d			(0.989) ^d					

Ne₂⁺: ^aFrom elastic scattering of Ne⁺ by Ne (3). A similar value ($D_0^0 = 1.35$ eV) from spectral line profiles in a Ne afterglow (dissociative recombination radiation of neon) is given by (1)(2). From ab initio theory (4) derive $D_e = 1.17$ eV.

^bTheoretical values (4).

- (1) Connor, Biondi, PR A 140, 778 (1965).
- (2) Frommhold, Biondi, PR 185, 244 (1969).
- (3) Mittmann, Weise, ZN 29 a, 400 (1974).
- (4) Cohen, Schneider, JCP 61, 3230, 3240 (1974).

NeAr: ^aFrom crossed-beam differential scattering measurements (4).

^bTheoretical values (5); the ground state potential supports four bound vibrational levels.

^cDipole moment function from ab initio calculations (2), from translational absorption spectra (3).

- (1) Bosomworth, Gush, CJP 43, 751 (1965).
- (2) Matcha, Nesbet, PR 160, 72 (1967).
- (3) Bar-Ziv, Weiss, CPL 12, 148 (1973).
- (4) Ng, Lee, Barker, JCP 61, 1996 (1974).
- (5) Bobetic, Barker, JCP 64, 2367 (1976).

NeAr⁺: ^aThe splittings between X_1 and X_2 and between A_2 and A_3 are very similar to those of the ²P ground states of Ar⁺ and Ne⁺ (1431 and 780 cm⁻¹, resp.). The splitting between A_1 and A_2 is molecular in nature; both states arise from ²P_{3/2} of Ne⁺ ($\Omega = 1/2$ and $3/2$). The corresponding splitting of X_1 is not resolved.

NeAr⁺ (continued):

^bThe transition energy $A_2 - X_1$ is close to the difference of Ne⁺ + Ar and Ne + Ar⁺ which is 46820 cm⁻¹. This agreement together with that mentioned in ^a makes the interpretation by (1) of the observed spectrum as a charge transfer spectrum very convincing.

(1) Tanaka, Yoshino, Freeman, JCP 62, 4484 (1975).

NeF: (1) Gardner, Karo, Wahl, JCP 65, 1222 (1976).

NeH, NeH⁺:

^aEnergies relative to Ne(¹S) + H(¹s²S). A, B, C have calculated dissociation energies D_e of 1.53, 1.50, 0.51 eV (5).

^bPredicted potential hump of 0.87 eV at 2.1 Å (5).

^cFrom a comparative study of the reactions $H_2^+ + He \rightarrow HeH^+ + H$ and $H_2^+ + Ne \rightarrow NeH^+ + H$ by photoionization mass-spectrometry (2); $D_0(NeH^+) - D_0(HeH^+) = +0.24$ eV. Theoretical values for D_e vary between 2.1 and 2.3 eV (1)(5)(6); similar values are obtained from proton scattering on Ne (3)(4).

^dTheoretical values (5).

- (1) Peyerimhoff, JCP 43, 998 (1965).
- (2) Chupka, Russell, JCP 42, 5426 (1968).
- (3) Rich, Bobbio, Champion, Doverspike, PR A 4, 2253 (1971).
- (4) Weise, Mittmann, Ding, Henglein, ZN 26 a, 1122 (1971).
- (5) Bondybey, Pearson, Schaefer, JCP 52, 1123 (1972).
- (6) Vasudevan, MP 30, 437 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
(20)Ne(84)Kr											
X $1\Sigma^+$	0	$(\mu = 16.1456407)$ [(18.7)] ^b		$D_e^0 = 0.0064 \text{ eV}^a$ $D_0^0 = (0.0048) \text{ eV}^b$			3.58 ^a			MAR 1977	
(20)Ne(84)Kr⁺											
A ₃ ($\frac{1}{2}$)	(60790) ^c	Five band groups [called A,B,C,D,E by (3)] with some vibrational structure which has, however, not been assigned.						A ₃ →X ₂	55310	(3)	
A ₂ ($\frac{3}{2}$)	(60020) ^c							A ₃ →X ₁	60790		
A ₁ ($\frac{1}{2}$)	(59770) ^c							A ₂ →X ₂	54560		
X ₂ ($\frac{1}{2}$)	(5470) ^c							A ₂ →X ₁	60020 ^d		
X ₁ ($\frac{1}{2}, \frac{3}{2}$)	0 ^c							A ₁ →X ₁	59770		
(20)Ne(132)Xe											
X $1\Sigma^+$	0	$(\mu = 17.3610604)$ [(17.5)] ^b		$D_e^0 = 0.0065 \text{ eV}^a$ $D_0^0 = (0.0048) \text{ eV}^b$			3.74 ₅ ^a	Translational sp.		MAR 1977 A (1)	
(20)Ne(132)Xe⁺											
A ₃ ($\frac{1}{2}$)	(75300) ^c	Five band groups [called A,B,C,D,E by (3)] with some vibrational structure which has, however, not been assigned.						A ₃ →X ₂	64730	(3)	
A ₂ ($\frac{3}{2}$)	(74520) ^c							A ₃ →X ₁	75300		
A ₁ ($\frac{1}{2}$)	(74460) ^c							A ₂ →X ₂	63940		
X ₂ ($\frac{1}{2}$)	(10575) ^c							A ₂ →X ₁	74520 ^d		
X ₁ ($\frac{1}{2}, \frac{3}{2}$)	0 ^c							A ₁ →X ₁	(74460)		
¹⁴N¹⁹F											
		$\mu = 8.0613378_9$		$D_0^0 = 3.5 \text{ eV}^a$							
Theoretical potential functions and spectroscopic constants for the ground and several excited states (5)(6)(8).											
b $1\Sigma^+$	18877.05	1197.49	Z	8.64	1.2377 ₀	0.01448	5.28	1.2998 ₃	b ^b →X, ^c v	18905.20 Z	(2)*
a 1Δ	[12003.60]				[1.2225] ^d		[4.5]	[1.3079]	a→X, v	11435.16 Z	(3)*
X $3\Sigma^-$	0	1141.37	Z	8.99	1.2056 ₈ ^e	0.01492	5.39	1.3169 ₈	Vibration sp. ^f		(1)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
NF ⁺ , NF ⁻		No experimental data; <u>ab initio</u> calculations (5)(6)(7a).								MAY 1977

NeKr, NeKr⁺;
NeXe, NeXe⁺;

^aFrom crossed-beam differential scattering measurements (2).

^bTheoretical values (4); the ground state potentials support five or possibly six (NeXe) bound vibrational levels.

^cThe splittings between X_1 and X_2 and between A_2 and A_3 are very similar to those of the 2P ground states of Kr⁺ (5371 cm^{-1}) or Xe⁺ (10537 cm^{-1}) and Ne⁺ (780 cm^{-1}). The splitting between A_1 and A_2 is molecular in nature; both states arise from $^2P_{3/2}$ of Ne⁺ ($\Omega = 1/2$ and $3/2$). The corresponding splitting in the ground state is not resolved.

^dThe transition energy $A_2 - X_1$ is close to the difference between the ionization potentials of Ne and Kr or Xe, i.e. 61015 or 76096 cm^{-1} . This agreement together with that mentioned in ^c makes the interpretation by (3) of the observed spectra as charge transfer spectra very convincing.

(1) Marteau, Granier, Vu, Vodar, CR B 265, 685 (1967).

(2) Ng, Lee, Barker, JCP 61, 1996 (1974).

(3) Tanaka, Yoshino, Freeman, JCP 62, 4484 (1975).

(4) Bobetic, Barker, JCP 64, 2367 (1976).

NF, NF⁺, NF⁻:

^aEstimated by (5) on the basis of spectroscopic and thermochemical data; the ab initio computed value is 3.6 eV.

^bLifetime 0.16 s, estimated from the rate of attenuation of the green emission in the reaction $N + NF_2$ along a flow

^cFranck-Condon factors (9). | tube (4).

^dThe EPR spectrum of NF($^1\Delta$) (7) yields $\mu_{el} = 0.37$ D as well as hyperfine coupling constants.

^eSpin coupling constants $\lambda_0 = 1.21_5$, $\gamma_0 = -0.0048$.

^fObserved in argon and nitrogen matrices, $\Delta G(\frac{1}{2}) = 1115$.

(1) Milligan, Jacox, JCP 40, 2461 (1964).

(2) Douglas, Jones, CJP 44, 2251 (1966).

(3) Jones, CJP 45, 21 (1967).

(4) Clyne, White, CPL 6, 465 (1970).

(5) O'Hare, Wahl, JCP 54, 4563 (1971); O'Hare, JCP 59, 3842 (1973).

(6) Andersen, Öhrn, JMS 45, 358 (1973).

(7) Curran, MacDonald, Stone, Thrush, PRS A 332, 355 (1973).

(7a) Ellis, Banyard, Tait, Dixon, JP B 6, L233 (1973).

(8) Ellis, Banyard, JP B 7, 2021 (1974).

(9) Mohamed, Khanna, Lal, IJPAP 12, 243 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^1\text{H}$		$\mu = 0.94016028$ $D_0^0 \leq 3.47 \text{ eV}^a$ I.P. = (13.63) eV^b								MAR 1977 A
Theoretical potential functions and spectroscopic constants for the ground and excited states: (21)(44)(46); (32)(36)(51).										
d $^1\Sigma^+$	83160	2672.6	Z	71.2	14.390 ^c	0.621	16.0 ^d	1.1163	$d^e \rightarrow c, ^m v$ 39512.2 ₆	Z (5)* (19) (23)(27) (55)*
c $^1\Pi$	(43744)	[2122.6 ₄]	Z	f	14.537 ^{ghi}	0.593 ^j	[22.0] ^k	1.110 ₆	$d^e \rightarrow b, ^m R$ 61619.6 ₀	Z (29)(55)*
									$c^l \rightarrow b, ^m R$ 22106.6 ₂	Z (4)* (26)*
									$c^l \rightarrow a, ^m R$ 30755.5 ₄	Z (1)(2)* (6) (14)*
A $^3\Pi_1$	29807.4 ⁿ	3231.2	Z	98.6	16.6745 ^{opi}	0.7454	[17.80] ^q	1.0369 ₈	$A^r \leftrightarrow X, ^m s$ 29776.76	Z (3)(8)* (18) (35)
b $^1\Sigma^+$	21202	3352.4	Z	74.2 ₄ ^t	16.705 ^u	0.591	16.0 ^v	1.0360	$b^w \rightarrow X, s$ 21238	Z (45)
a $^1\Delta$	(12566) ^x	[3188]	Z	(68) ^y	[16.439] ⁱ	0.66	[16.2]	1.034 ₁	(a-X) 12589 ^z	
X $^3\Sigma^-$	0	3282.2 ₇	Z	78.3 ₅	16.6993 ^{a'}	0.6490	[17.097] ^{b'}	1.0362 ₁	Rotation sp. ^{c'}	(48)(54)
Fundamental b. in matrices (45a)(55a)										

N^1H : ^aFrom the limiting curve of dissociation in c $^1\Pi$ (55), see ^h and ^f. Theoretical calculations by (33)(39)(43) suggest $D_0^0 = 3.43, 3.31, 3.17 \text{ eV}$, resp.; the most recent prediction on theoretical and empirical grounds (46) is $D_0^0 = 3.40 \text{ eV}$. From the electron impact appearance potential of N_2^+ from HN_3 (7) follows $D_0^0 = 3.59 \text{ eV}$; a shock-tube measurement (20) gives 3.2_1 eV . Both results are compatible with limits derived from the study of reactions of rare gas metastables with small NH-containing molecules (31), the upper limit being closer to the semi-empirical calculations of (10)(12), the lower limit being in better agreement with the thermochemical measurements of (38).

^bTheoretical value (33); (16) give an electron impact appearance potential of 13.1 eV.

^c(27) report a breaking-off in the $d \rightarrow c$ 1-1 band above $J'=15$ which they attribute to predissociation in the upper state. Intensity anomalies are confirmed (55) for the $d \rightarrow c$ 1-1 and 1-0 bands, but higher rotational levels (except $J'=16$) do emit in transitions to the b state (55). Similar intensity perturbations are seen in other $d \rightarrow b$ and $d \rightarrow c$ bands.

^d $H_e = +10 \times 10^{-8}$.

^eRadiative lifetime $\tau(v=0) = 18 \text{ ns}$ (28).

^f $\Delta G(3/2) = 1694.0_8$. The theoretical calculations of (32) predict a potential maximum resulting from the avoided

N^1H (continued):

crossing of the two 1Π states arising from $N(^2D) + H(^2S)$ and $N(^2P) + H(^2S)$.

^g Λ -type doubling $\Delta v_{ef}(v=0) = +0.0165 J(J+1)$.

^hPredissociation by rotation in $v=0$ above $J=22$ and in $v=1$ above $J=15$ (27)(55). A much weaker predissociation, not seen on the photographic plates but detected by high-resolution lifetime measurements [(50), see ^l], affects the lower J levels of both $v=0$ and 1 and may be caused by interaction with the unstable $^5\Sigma^-$ state arising from ground state atomic products. All rotational structure in $v=2$ is diffuse except for $J=1$.

ⁱElectric dipole moments of a 1Δ , A 3Π , c $1\Pi = 1.49, 1.31, 1.70$ D, respectively (15); see also (25).

^j $\gamma_e = -0.347$ (55).

^k $D_1 = 26.6 \times 10^{-4}$, $D_2 = 51.0 \times 10^{-4}$; $H_0 = -26 \times 10^{-8}$, $H_1 = -115 \times 10^{-8}$ (55).

^lLifetime $\tau(v=0, J=2) = 411$ ns (50), decreasing with increasing rotation to 226 ns for $J=17$ owing to weak predissociation; in $v=1$ the longest lifetime (57.1 ns) was observed (50) for $J=4$. See also (13)(28) whose low-resolution measurements gave $\tau(v=0) \approx 460$ ns. Relative transition probabilities (41).

^mFranck-Condon factors (37)(42).

ⁿ $A(v=0, 1) = -34.79$; from (40) who gives also spin-spin and spin-rotation interaction constants. See also (22)(30).

^o"True" rotational constants of (40); see also (22)(30).

Λ -type doubling parameters may be found in (22)(40). The effective constants (18) are $B_e = 16.6901$, $\alpha_e = 0.7440$.

^pWeak predissociation in $v=0$ and 1 above $N=25$ and 15 , resp., observed by high-resolution lifetime measurements (50) and attributed to interaction with the unstable $^5\Sigma^-$ state arising from $^4S + ^2S$.

$q + 9.9 \times 10^{-8} J^3(J+1)^3 - 13 \times 10^{-12} J^4(J+1)^4$; $D_1 = 17.85 \times 10^{-4}$, $H_1 = +6.0 \times 10^{-8}$ (40).

^rLifetime $\tau(v=0, N=4) = 404$ ns (50), first increasing to 453 ns at $N=25$, then decreasing rapidly to 96 ns at $N=31$ owing to predissociation. Similar results for $v=1$, see ^p. Absorption oscillator strength 0.0076 (11)(13)(28); f values in (17) refer to emission and should be multiplied by 2 for comparison. Relative transition probabilities (41).

^sUndegraded 0-0 band.

^t $w_e y_e = +0.70$, $w_e z_e = -0.035_3$ ($v \leq 9$).

^uRotational constants from the analysis of the $d \rightarrow b$ bands [(55), $1 \leq v \leq 9$]. (26) gives $B_e = 16.7326$ and $\alpha_e = 0.6049$ from the $c \rightarrow b$ 0-0 and 0-1 bands.

^v $H_e = 11 \times 10^{-8}$.

^wRadiative lifetime $\tau = 18$ ms (47)(49).

^xEarlier theoretical predictions by (9) and (24) gave 14200 and 13100 cm^{-1} , respectively.

^yFrom a comparison with $\Delta G(\frac{1}{2})$ of ND.

^z $v_{00}(b-X) + v_{00}(c-b) - v_{00}(c-a)$; in very good agreement with the singlet-triplet separation of 12500 cm^{-1} derived by (34) from the difference of the threshold energies for the production of $NH(c^1\Pi) + CO(X^1\Sigma)$ or $NH(X^3\Sigma) + CO(a^3\Pi)$ by photodissociation of HNC. From the photoelectron spectrum of NH^- (53) find 12735 \pm 137 cm^{-1} .

^a"True" rotational constants of (40); spin-splitting constants $\gamma = -0.011_7$, $\lambda \approx +0.82$. The evaluation of the constants by (40) takes fully into account the $^3\Pi \sim ^3\Sigma^-$ interaction and thus leads to results which differ considerably from the effective constants of earlier investigators (8)(18)(30)(35). The latter are in good agreement with more precise constants obtained recently from the laser-magnetic- (continued on p. 459)

State	T _e	w _e		w _e x _e	B _e	α _e	D _e (10 ⁻⁴ cm ⁻¹)	r _e (Å)	Observed Transitions		References
									Design.	v ₀₀	
¹⁴ N ² H		μ = 1.76083613		D ₀ ⁰ ≤ 3.54 eV ^a						MAR 1977 A	
d	¹ Σ ⁺	83168	1953.7	Z	38.2	7.693	0.257 ^b	[4.81] ^b	1.1156	d → c, V 39484.22 Z	(8)* (16)
										d → b, R 61721.5 (Z)	(10)
c	¹ Π	43786	1756.5	Z	50.9 ₅ ^c	7.833 ^{de}	0.379 ^f	[6.07] ^g	1.105 ₅	c → b, R 22237.3 ₁ Z	(9)*
										c ↔ a, ^h R 30849.0 ₆ Z	(1)(2)(3)* (4)*
A	³ Π _i	29820 ⁱ	2361 ^j		53 ^j	[8.7575] ^k	0.282 ₉ ^l	[5.08 ₇] ^k	1.0372	A ↔ X, ^m 29798.7 ₅ Z	(3)* (5)(6) (7)(11)*
b	¹ Σ ⁺	21198	[2371.8 ₁]	Z	38.8 ⁿ	8.947 ₂	0.238 ₃	4.6 ₄	1.0344	b → X, ^m 21225 Z	(14)
a	¹ Δ	(12596)	[2356.1 ₇]	Z	(36) ^o	8.954 ₂	0.242 ₇	[4.83 ₈] ^p	1.0340	(a-X) 12613 ^q	
X	³ Σ ⁻	0	2398 ^j		42 ^j	[8.7913] ^r	0.2531 ^s	[4.904] ^r	1.0361 ₂	Rotation sp. ^t	(15)

N^2H : ^aFrom the limiting curve of dissociation in c 1Π (16); see ^e. See also ^f of NH.
^b $\gamma_e = +0.0033$ ($v=0,1,2$), $B_3 = 6.864$; $D_{1,2,3}(10^{-4} \text{ cm}^{-1}) = 4.50, 4.51, 12$; $H_0 = +2.49 \times 10^{-8}$ (16).
^c $w_e v_e = -10.3_7$.
^d Λ -type doubling $\Delta v_{ef}(v=0) = +0.00436 \text{ J}(J+1)$, and increasing with v (8)(16).
^ePredissociation by rotation in $v=0\dots 3$ above $J=30, 25, 18, 5$, respectively (16).
^f $\gamma_e = -0.047$ ($v \leq 2$); $B_3 = 5.80_3$ (16).
^g $D_{1,2,3}(10^{-4} \text{ cm}^{-1}) = 6.49, 8.06, 27$;
 $H_{0,1,2}(10^{-8} \text{ cm}^{-1}) = -4.0, -13.2, -38.5$.
^hObserved in absorption by (11) in the flash photolysis of DN_3 .
ⁱ $A_0 = -34.58$; from (13) who gives additional multiplet splitting constants. See also (12).

^jCalculated from the constants for N^1H . The origins of the A \leftrightarrow X 1-1 and 2-2 bands are at 29738.4_2 and $29658.1_9 \text{ cm}^{-1}$.
^k"True" constants calculated by (13) from the data of (11), $H_0 = +1.57 \times 10^{-8}$. The Λ -type doubling parameters were also evaluated by (13). $B_0(\text{effective}) = 8.7610 \text{ cm}^{-1}$ (6); for effective D_v, H_v values ($v=0,1,2$) see (6)(7).
^l $\gamma_e = -0.003_3$. α_e and γ_e refer to the effective rotational constants of (6)(7).
^mUndegraded 0-0 band.
ⁿAverage of two values obtained a) from $w_e x_e$ of N^1H and b) from bandhead measurements and calculated head-origin separations in the d \rightarrow b system.
^oFrom a comparison with $\Delta G(\frac{1}{2})$ of N^1H .
 $P_{D1} = 4.71 \times 10^{-4}$, $H_0 = +2.09 \times 10^{-8}$.
^q $v_{00}(b-X) + v_{00}(c-b) - v_{00}(c-a)$.
^r"True" B_0 and D_0 from (13), $H_0 = +1.82 \times 10^{-8}$; multiplet (continued on p. 461)

N^1H (continued):

resonance spectrum (54) in $v=0$ and 1; $B_e = 16.6668$, $\alpha_e = 0.6470$; $\gamma(v=0) = -0.05466$, $\gamma(v=1) = -0.0517$; $\lambda(v=0,1) = +0.9198$. See also (52).

^b $D_1 = 16.88 \times 10^{-4}$, $H_0 = +10.48 \times 10^{-8}$, $H_1 = +10.2 \times 10^{-8}$ (40).

^c By the laser-magnetic-resonance method; fine (see ^a) and hyperfine structure constants.

- (1) Dieke, Blue, PR 45, 395 (1934).
- (2) Pearse, PRS A 143, 112 (1934).
- (3) Funke, ZP 96, 787 (1935); 101, 104 (1936).
- (4) Lunt, Pearse, Smith, PRS A 151, 602 (1935).
- (5) Lunt, Pearse, Smith, PRS A 155, 173 (1936).
- (6) Florent, Leach, JPR 13, 377 (1952).
- (7) Franklin, Dibeler, Reese, Krauss, JACS 80, 298 (1958).
- (8) Dixon, CJP 37, 1171 (1959).
- (9) Hurley, PRS A 249, 402 (1959).
- (10) Companion, Ellison, JCP 32, 1132 (1960).
- (11) Bennett, Dalby, JCP 32, 1716 (1960).
- (12) Jordan, Longuet-Higgins, MP 5, 121 (1962).
- (13) Fink, Welge, ZN 19 a, 1193 (1964).
- (14) Shimauchi, SL 13, 53 (1964).
- (15) Irwin, Dalby, CJP 43, 1766 (1965).
- (16) Foner, Hudson, JCP 45, 40 (1966).
- (17) Harrington, Modica, Libby, JQSRT 6, 799 (1966).
- (18) Murai, Shimauchi, SL 15, 48, 165(erratum) (1966).
- (19) Narasimham, Krishnamurty, PIAS A 64, 97 (1966).
- (20) Seal, Gaydon, PPS 89, 459 (1966).
- (21) Cade, Huo, JCP 47, 614 (1967).
- (22) Horani, Rostas, Lefebvre-Brion, CJP 45, 3319 (1967).
- (23) Whittaker, PPS 90, 535 (1967).
- (24) Cade, CJP 46, 1989 (1968).
- (25) Huo, JCP 49, 1482 (1968).

- (26) Whittaker, JP B 1, 977 (1968).
- (27) Krishnamurty, Narasimham, JMS 29, 410 (1969).
- (28) Smith, JCP 51, 520 (1969).
- (29) Whittaker, CJP 47, 1291 (1969).
- (30) Bollmark, Kopp, Rydh, JMS 34, 487 (1970).
- (31) Stedman, JCP 52, 3966 (1970).
- (32) Kouba, Öhrn, JCP 52, 5387 (1970).
- (33) Liu, Verhaegen, JCP 53, 735 (1970).
- (34) Okabe, JCP 53, 3507 (1970).
- (35) Malicet, Brion, Guénébaut, JCPPB 67, 25 (1970).
- (36) O'Neil, Schaefer, JCP 55, 394 (1971).
- (37) Smith, Liszt, JQSRT 11, 45 (1971).
- (38) Kaskan, Nadler, JCP 56, 2220 (1972).
- (39) Liu, Legentil, Verhaegen, in "Selected Topics in Molecular Physics"(ed. Clementi), p.19. Chemie GmbH (1972).
- (40) Veseth, JP B 5, 229 (1972).
- (41) Lents, JQSRT 13, 297 (1973).
- (42) Rao, Lakshman, IJPAP 11, 539 (1973).
- (43) Stevens, JCP 58, 1264 (1973).
- (44) Das, Wahl, Stevens, JCP 61, 433 (1974).
- (45) Gilles, Masanet, Vermeil, CPL 25, 346 (1974); JPhOC 3, 417 (1974/75).
- (45a) Milligan, Jacox, JCP 41, 2838 (1964).
- (46) Meyer, Rosmus, JCP 63, 2356 (1975).
- (47) Zetzsch, Stuhl, CPL 33, 375 (1975).
- (48) Radford, Litvak, CPL 34, 561 (1975).
- (49) Gelernt, Filseth, Carrington, CPL 36, 238 (1975).
- (50) Smith, Brzozowski, Erman, JCP 64, 4628 (1976).
- (51) Hay, Dunning, JCP 64, 5077 (1976).
- (52) Palmiere, Sink, JCP 65, 3641 (1976).
- (53) Engelking, Lineberger, JCP 65, 4323 (1976).
- (54) Wayne, Radford, MP 32, 1407 (1976).
- (55) Graham, Lew, CJP 56, 85 (1978).
- (55a) Rosengren, Pimentel, JCP 43, 507 (1965).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (Å)	Observed Transitions		References	
								Design.	v_{00}		
$^{14}\text{N}^1\text{H}^+$		$D_0^0 = (3.39) \text{ eV}^a$ <u>Ab initio</u> calculated potential energy curves for the ground and excited states (3).							MAR 1977		
C	$2\Sigma^+$ (35000)	2150.5 ₆	Z	73.0 ₇	13.265 ₂ ^b	0.789 ₁ ^c	20.0 ^d	1.1626	$C^{\dagger} \rightarrow X$, R	34561.27 ^e	(1)* (2)(5)*
B	$2\Delta_i$ (23300) ^f	(2280)			[13.516]		[19]	[1.1518]	$B^{\dagger} \rightarrow X$, R	22960.46 ^e	(2)*
A	$2\Sigma^-$ (22200)	[1585.49]	Z	(61) ^g	11.4553 ^h	0.6897	[20.2] ⁱ	1.2511	$A^{\dagger} \rightarrow X$, R	21567.67 ^e	(2)*
a	$4\Sigma^-$ (500)	[2520] ^j			[14.69] ^j		(17)	[1.105]	(a-X)	354 ^{e,j}	
X	$2\Pi_r$ 0 ^k	[2922] ^l			[15.35] ^{lm}	(0.64) ^l	[17] ^l	1.070			
$^{14}\text{N}2\text{H}^+$										MAR 1977	
B	$2\Delta_i$ (23300) ⁿ	(1672)			[7.2715]		[5.5] ^o	[1.1474]	$B \rightarrow X$, R	23063.83 ^e	(2)
A	$2\Sigma^-$ (22200)	[1182.40]	Z	(32) ^g	6.1206 ^p	0.2752	[5.8] ^q	1.2507	$A \rightarrow X$, R	21750.59 ^e	(2)
X	$2\Pi_r$ 0 ^r	[2143.04]	Z		[8.244]	^s	[5.3]	[1.077 ₆]			
$^{14}\text{N}^1\text{H}^-$		$\text{I.P.} = 0.38_1 \text{ eV}^a$								MAR 1977	
X	$2\Pi_i$ 0 ^b							1.047 ^c			
$^{14}\text{N}^{127}\text{I}$		$\mu = 12.6114804_6$								MAY 1977	
X	$3\Sigma^-$ 0	[590] ^a							Vibrational sp. ^a		(1)

N^1H^+ , N^2H^+ .

^aTheoretical value (3), corresponding to $\text{N}(^4\text{S}) + \text{H}^+$. The 2Π ground state must dissociate into $\text{N}^+(^3\text{P}) + \text{H}(^2\text{S})$.

^bSpin-splitting constants $\gamma_0 \dots \gamma_2 = +0.105, +0.108, +0.111$.

^c $\gamma_e = +0.008_9$.

^d $\beta_e \approx -0.8 \times 10^{-4}$, $H_e \approx +11 \times 10^{-8}$.

^eEnergy of lowest rotational level relative to the lowest level [$F_{1e}(\frac{1}{2})$] of the ground state.

^f $A_0 = -3.6$.

N^1H^+ , N^2H^+ (continued):

^gEstimated from the $\Delta G(\frac{1}{2})$ values for NH^+ and ND^+ .

^hSpin-splitting constants $\gamma_0 = -0.097$, $\gamma_1 = -0.100$.

ⁱ $D_1 = 18.6 \times 10^{-4}$, $H_0 = +18.5 \times 10^{-8}$.

^jFrom the analysis of perturbations in $X^2\Pi(v=0,1)$ (2).

^k $A_0 = +77.8$.

^l $v=0,1$ strongly perturbed by $v=0,1$, resp., of a $4\Sigma^-$ (2)(5).

^m Λ -doubling in $2\Pi_{1/2}(v=0, J=\frac{1}{2})$: $\Delta v_{fe} = +0.451 \pm 0.010 \text{ cm}^{-1}$.

ⁿ $A_0 = -3.5$.

^o $H_0 = +1.5 \times 10^{-8}$.

^pSpin-splitting constants $\gamma_0 = -0.052$, $\gamma_1 = -0.053$.

^q $D_1 = 5.5 \times 10^{-4}$.

^r $A_0 = +78.4$.

^s $v=1$ strongly perturbed by $v=1$ of a $4\Sigma^-$.

^tLifetimes of A, B, C: 1.0₉, 0.9₈, 0.40 μ s, resp. (4).

(1) Feast, ApJ 114, 344 (1951).

(2) Colin, Douglas, CJP 46, 61 (1968).

N^2H (continued):

splitting parameters $\lambda_0 \approx +0.89_5$, $\gamma_0 = -0.0061$. The evaluation of these constants (13) takes fully into account the $3\Pi \sim 3\Sigma^-$ interaction and thus gives results that differ considerably from the effective constants (5)(6)(11). The latter are in good agreement with the more precise constants from the laser-magnetic-resonance sp. (15): $B_0 = 8.7815$, $\lambda_0 = +0.9184$, $\gamma_0 = -0.0294$. Effective D_v , H_v values in (6)(7).

^sFrom the effective B_v values (5)(6)(7).

^tLaser magnetic resonance; hyperfine structure constants.

(1) Dieke, Blue, PR 45, 395 (1934).

(2) Florent, Leach, JPR 13, 377 (1952).

(3) Shimauchi, SL 13, 53 (1964).

N^1H^+ , N^2H^+ (continued):

(3) Liu, Verhaegen, JCP 53, 735 (1970).

(4) Brzozowski, Elander, Erman, Lyyra, PS 10, 241 (1974).

(5) Krishnamurthy, Saraswathy, Pramāṇa 6, 235 (1976).

NH^- : ^aFrom the laser photodetachment spectrum (1)(2).

^b $A = -63 \text{ cm}^{-1}$ [estimated (2)].

^cFrom a Franck-Condon factor analysis of the observed $3\Sigma^- \leftarrow 2\Pi$ photoelectron spectrum (2).

(1) Celotta, Bennett, Hall, JCP 60, 1740 (1974).

(2) Engelking, Lineberger, JCP 65, 4323 (1976).

NI : ^aObserved in the condensate at 10 K of the products of a discharge in an N_2/I_2 mixture. The observation of a corresponding band at 573 cm^{-1} for ^{15}NI supports the assignment.

(1) Minkwitz, Froben, CPL 39, 473 (1976).

(4) Hanson, Kopp, Kronekvist, Åslund, AF 30, 1 (1965).

(5) Kopp, Kronekvist, Åslund, AF 30, 9 (1965).

(6) Shimauchi, SL 15, 161 (1966).

(7) Shimauchi, SL 16, 185 (1967).

(8) Whittaker, PPS 20, 535 (1967).

(9) Whittaker, JP B 1, 977 (1968).

(10) Whittaker, CJP 47, 1291 (1969).

(11) Bollmark, Kopp, Rydh, JMS 34, 487 (1970).

(12) Kovács, Korwar, APH 29, 85 (1970).

(13) Veseth, JP B 5, 229 (1972).

(14) Gilles, Masanet, Vermeil, CPL 25, 346 (1974); JPhoC 3, 417 (1974/75).

(15) Wayne, Radford, MP 32, 1407 (1976).

(16) Graham, Lew, CJP 56, 85 (1978).

System	ν_e	ω_e'	$\omega_e'x_e'$	ω_e''	$\omega_e''x_e''$	Remarks Description	Degrad.	ν_{00}	References
(58)Ni₂		$(\mu = 28.967667_9)$ $D_0^0 = 2.3_6 \text{ eV}^a$ Absorption in the region $21790 - 23900 \text{ cm}^{-1}$; in Ar matrices at 10 K. $\omega' \approx 192 \text{ cm}^{-1}$.							MAR 1976 A (2)
(58)Ni⁽⁷⁹⁾Br		$(\mu = 33.409116_0)$ $D_0^0 = 3.6_9 \text{ eV}^a$ Large number of R shaded emission bands in the region $20000 - 25600 \text{ cm}^{-1}$. Below are preliminary assignments by (3):							MAR 1975
System α_1 :	24326.2	297.0	H ^R 3.35	311.6	1.7	R, Q heads. b	R	24318.5 ^C H ^R	(3)* (5)
" α_2 :	23920.3	262	H	293.2		b	R	23904.7 H	(3)
" α_3 :	23791.1	305.4	H ^R 0.2	315.0	0.5	R, Q(?) heads. d	R	23786.4 H ^R	(3)
" β_1 :	22975.5	293.8	H 2.5	322.8	1.0	b	R	22960.6 H	(3)* (5)
" β_2 :	22435.9	257	H ^Q	274		d	R	22427.4 H ^Q	(3)*
" γ :	21792.6	297.5	H ^Q 1.1	323.0	1.2	b	R	21779.9 H ^Q	(3)
(58)Ni⁽³⁵⁾Cl		$(\mu = 21.806683_7)$ $D_0^0 = 3.8_2 \text{ eV}^a$ Large number of R shaded emission bands in the regions $11000 - 15000$ and $18000 - 26000 \text{ cm}^{-1}$. The ground state has not been identified and all assignments must be considered as preliminary.							MAR 1975
System A_1 :	24623.7	394.5	H ^Q 0.35	415.5	1.3	b	R	24613.4 H ^Q	(1)(4)*
" A_2 :		0-0 sequence only.				g	R	24411.6 H ^Q	(1)(2)(4)*
" A_3 :	24138.3	380	H	397		c	R	24129.8 H	(1)(4)*
" B_1 :	23347.1	375	H	402		d	R	23333.6 H	(4)
" B_2 :	23233.1	406.6	H 2.75	426.3	1.9	e	R	23223.0 H	(1)(2)(4)*
" C :	22749.0	397.8	H ^Q 0.75	418.2	0.70	f	R	22738.8 H ^Q	(1)(2)(4)*
" D :	21914.7	398	H ^Q	417		g	R	21905.2 H ^Q	(4)*
" E_1 :	21762.2	405.2	H 1.3	435.3	1.85	g	R	21747.3 H	(4)*
" E_2 :	21649.4	383.1	H ^Q	404.0	1.65	g	R	21639.4 H ^Q	(4)*
" I :	20545.3	409.6	H ^Q 0.80	431.1	0.20		R	20534.4 H ^Q	(7)
" II :	20284.2	382.8	H ^Q	423.9	1.35		R	20264.0 H ^Q	(7)
" III :	19980.1	403.6	H ^Q 0.05	430.0	0.30		R	19967.0 H ^Q	(7)

System	ν_e	ω_e	$\omega_e'x_e'$	ω_e''	$\omega_e''x_e''$	Remarks Description			References
							Degrad.	ν_{00}	
(58)Ni(35)Cl (continued)									
System IV:	18689.4	412.6	H 1.60	433.2	1.65	h h	R	18679.1 H	(7)
" F:	14441.2	407.2	H 2.5	420			R	14434.2 H	(6)
" G:	12976.5	395.0	H 1.55	424			R	12961.6 H	(6)
" H:	12276.8	416.0	H ^Q	428			R	12270.8 H ^Q	(6)
" I:	11913.1	395.0	H 1.40	402			R	11909.3 H	(6)
" J:	11511.3	398.7	H ^Q 1.45	405.2	1.15		R	11508.0 H ^Q	(6)

Ni₂: ^aThermochemical value (mass-spectrom.)(1).
 (1) Kant, JCP 41, 1872 (1964).
 (2) De Vore, Ewing, Franzen, Calder, CPL 35, 78 (1975).
 NiBr: ^aThermochemical value (flame photometry)(4).
^bAlternative assignments in (1)(2).
^cQ head at 24311.9 cm⁻¹.
^dAlternative assignments in (1)(2)(5).
 (1) Mesnage, AP(Paris) 12, 5 (1939).
 (2) Krishnamurty, IJP 26, 429 (1952).
 (3) Reddy, Rao, PPS 75, 275 (1960).
 (4) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
 (5) Sundarachary, PNASI A 32, 311 (1962).

NiCl: ^aThermochemical value (flame photometry)(5).
^bSystem 4 of (1). Alternative assignments in (3).
^cSystem 3 of (1). Alternative assignments in (2)(3).
^dAlternative assignments in (2)(3).
^eSystem 2 of (1). Alternative assignments in (3).
^fSystem 1 of (1). Alternative assignments in (3).
^gAlternative assignments in (3).
^hResults of a rotational analysis in (7). Uncertain.
 (1) More, PR 54, 122 (1938).
 (2) See ref. (1) of NiBr.
 (3) Krishnamurty, IJP 26, 207 (1952).
 (4) See ref. (3) of NiBr.
 (5) See ref. (4) of NiBr.
 (6) Rao, Reddy, Rao, ZP 166, 261 (1962).
 (7) Rao, Rao, CS 38, 589 (1969).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(58)Ni ¹⁹ F		$(\mu = 14.3068431)$ Fragments of a band system. (740)						A \rightarrow (X), 22144 H		APR 1975 (1)
(58)Ni ⁽⁷⁴⁾ Ge		$(\mu = 32.479611_1) \quad D_0^0 = 2.8_8 \text{ eV}^a$								APR 1975
(58)Ni ¹ H		$(\mu = 0.99059317) \quad D_0^0 \leq 3.07 \text{ eV}^a$ Diffuse R shaded head in absorption at 34073 cm^{-1} .								APR 1975 (6)*
$C_2 \quad 2\Delta_{3/2}$	e			$[6.31_1]^{bc}$	$[7.6]$	$[1.642]$	$C_2 \leftarrow X_2, R$	23100.80^{dz}	(4)(5)	
$C_1 \quad 2\Delta_{5/2}$				$[6.156]^{bf}$	$[6.1]$	$[1.662_7]$	$C_2 \leftarrow X_1, R$	24081.2_3^{dz}		
B $2\Delta_{5/2}$		16193	1570.9 Z 34.55 ^g	h			$C_1 \leftrightarrow X_1, R$	23760.7^{dz}		(2)* (4)(5)
A $2\Delta_{5/2}$				$[6.283]^i$	$[4.7_5]$	$[1.645_8]$	A $\leftrightarrow X_1, R$	15977.3^{dz}		(1)* (2)(3) (6)
$X_2 \quad 2\Delta_{3/2}$	(980) j			$[7.781]^b$	$[5.9]$	$[1.4789]$	A $\leftrightarrow X_1, R$		15520.1^{dz}	(1)* (2)(3) (6)
$X_1 \quad 2\Delta_{5/2}$		0	$[1926.6] \quad Z \quad (38)^k$	$[7.700]^b$	0.23_1^l	$[4.81]^l$				
(58)Ni ² H		$(\mu = 1.94643507) \quad D_0^0 \leq 3.10 \text{ eV}^a$ Diffuse R shaded head in absorption at 34073 cm^{-1} .								APR 1975 (6)*
$C_2 \quad 2\Delta_{3/2}$	$C_1 \quad 2\Delta_{5/2}$	$[728.9_7]^m \quad Z$		$[3.271]$	mn	$[1.62]^m$	$[1.627_2]$	$C_2 \leftarrow X_2, R$	23171.6_9^{dz}	(4)(5)
		$[918.3_0] \quad Z$		$[3.240]$	0.188^n	$[1.52]^o$	1.611_7	$C_1 \leftarrow X_1, R$	23830.4_7^{dz}	(4)(5)
		R shaded absorption bands with heads at 19707 and 19845 cm^{-1} . Perturbations.								(6)*
B $2\Delta_{5/2}$	16172	1130.0 Z 23.4	p				B $\leftarrow X_1, R$	16021.8^{dz}		(6)*
$X_2 \quad 2\Delta_{3/2}$	(980)			$[3.996]$		$[1.42]$	$[1.472_2]$			
$X_1 \quad 2\Delta_{5/2}$	0	$[1390.0_9] \quad Z \quad (19)^k$	$[3.992]$	0.092	$[1.30]^q$	1.464_5				

NiF: (1) Krishnamurty, IJP 27, 354 (1953).

NiGe: ^aThermochemical value (mass-spectrom.)(1).

(1) Kant, JCP 44, 2450 (1966).

Ni¹H, Ni²H:

^aFrom the predissociation in C₁.

^bFor Λ -type doubling see (5).

^cLines with $J' \geq 11\frac{1}{2}$ are diffuse.

^dThese band origins are corrected for J-independent terms not usually taken into account in these tables.

^eA₀ = - 160.2 + ...

^fLines with $J' \geq 12\frac{1}{2}$ are diffuse, both in absorption and in thermal emission.

^g $\epsilon_{we} y_e = - 2.87$; from $v=0$, ..., 3 only. See ^h.

^hAll observed levels perturbed. Heimer (2)(3) obtained the following B_v values by extrapolation to J=0:

v = 0, B _v = 5.113 (increasing with J),
1 5.350 (" " J),
2 5.480 (" " J),
3 5.900 (decreasing with increasing J).

A reanalysis of the red band systems of NiH is considered necessary by (5).

Ni¹H, Ni²H (continued):

ⁱ Λ -type doubling increases rapidly above $J=9\frac{1}{2}$.

See (2).

^jA₀ = - 490.2 + ...

^kFrom isotope relations.

^lD₁ = 7.8×10^{-4} . Heimer (2)(3) finds $\alpha_e = 0.248$, D₁ = 5.1×10^{-4} , but his interpretation of a perturbation in the 0-1 band of C₁-X₁ is questioned by (5).

^mIt is not certain that the level assigned as v=1 (B₁ = 3.410, D₁ = 3.6×10^{-4}) belongs to the same electronic state.

ⁿLines of the 1-0 band with $J' \geq 9\frac{1}{2}$ are broad.

^oD₁ = 2.0×10^{-4} .

^pAll observed levels perturbed. Extrapolation to J=0 gives B₀ = 2.930, B₁ = 2.710, B₂ = 2.463.

^qD₁ = $1.4_0 \times 10^{-4}$.

(1) Gaydon, Pearse, PRS A 148, 312 (1935).

(2) A. Heimer, Dissertation (Stockholm, 1937).

(3) Heimer, ZP 105, 56 (1937).

(4) Andersén, Lagerqvist, Neuhaus, Åslund, PPS 82, 637 (1963).

(5) Åslund, Neuhaus, Lagerqvist, Andersén, AF 28, 271 (1964).

(6) Smith, PRS A 332, 113 (1973).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(58)Ni ¹²⁷ I		$(\mu = 39.776352_0) \quad D_0^0 = 2.9_9 \text{ eV}^a$							APR 1975	
(58)Ni ¹⁶⁰		$(\mu = 12.5343923_8) \quad D_0^0 = 3.8_7 \text{ eV}^a$ Three additional systems in the same spectral region.							APR 1975	
b	a + (21262)	(570)	H					b → a,	R (21135) H	(1)(2)
a	a	(825)	H							(1)(2)
B	(16447)	(560)	H					B → X,	R (16420) H	(1)(2)
A	(12725)	(475)	H					A → X,	R (12655) H	(1)(2)
(X)	0	(615)	H							
(58)Ni ⁽³²⁾ S		$(\mu = 20.6024487) \quad D_0^0 = 3.5_3 \text{ eV}^a$							APR 1975	
(58)Ni ⁽²⁸⁾ Si		$(\mu = 18.8663722) \quad D_0^0 = 3.2_6 \text{ eV}^a$							APR 1975	
¹⁴ N ¹⁶⁰		$\mu = 7.46643323 \quad D_0^0 = 6.496_8 \text{ eV}^a \quad \text{I.P.} = 9.26436 \text{ eV}^b$							MAR 1977 A	

For a detailed discussion of the electronic spectrum with particular emphasis on Rydberg~Rydberg and Rydberg~non-Rydberg interactions see (192a); this review contains references to spectra of four isotopes as well as a short summary of theoretical calculations.

$(^2\Sigma^-, ^2\Delta, ^2\Sigma^+)$	Broad unresolved peak in the oxygen K shell electron energy loss spectrum at 532.7 eV. ^c	(182a)
$(^2\Sigma^-)$	Rydberg states converging to the nitrogen K edge at 410.2 (³ Π) and 411.7 (¹ Π) eV, observed in X-ray absorption and electron energy loss spectra at 406.3, 407.3, 408.6 eV, ...	(178)(182a)
$(^2\Delta, ^2\Sigma^+, ^2\Sigma^-)$	Two very weak bands in the X-ray absorption spectrum at 402.3 and 403.9 eV. ^d	(178)
$(^2\Sigma^-, ^2\Delta, ^2\Sigma^+)$	Strong unresolved peak in X-ray absorption and electron energy loss spectra at 399.8 eV. ^e	(178)(182a)

NiI: ^aThermochemical value (flame photometry)(1).
(1) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

NiO: ^aThermochemical value (mass-spectrom.)(5), recalc. (6).
See also (3)(4).
(1) Rosen, Nature 156, 570 (1945).
(2) Malet, Rosen, BSRSL 14, 382 (1945).
(3) Brewer, Mastick, JCP 19, 834 (1951).
(4) Huldt, Lagerqvist, ZN 2 a, 358 (1954).
(5) Grimley, Burns, Inghram, JCP 35, 551 (1961).
(6) Smoes, Mandy, Vander Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

NiS: ^aThermochemical value (mass-spectrom.)(1).
(1) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).

NiSi: ^aThermochemical value (mass-spectrom.)(1).
(1) Vander Auwera-Mahieu, McIntyre, Drowart, CPL 4, 198 (1969).

NO: ^aFrom the breaking-off below $N'=4$ in the C→A O-O band emitted during radiative recombination of N and O atoms via inverse predissociation (187), see also (169); in good agreement with (123). A very slightly higher value, i.e. $6.4977 \leq D_0^0 \leq 6.5007$ eV, is suggested (179) by the failure to detect F→C laser transitions ending on the lowest C level observed in the N+O recombination spectrum.

^bExtrapolation of selected rotational lines in the $nf \leftarrow X$ Rydberg series (180)(204), based on the fine structure analysis of the 4f and 5f complexes (119).

^cExcitation of a $1s_0$ electron to the 2π orbital.

^dTentatively interpreted as arising from two-electron excitation from the $1s_N$ and 1π to the 2π orbital (178). Only one peak (404.7 eV) is observed in the electron energy loss spectrum (182a).

^eExcitation of a $1s_N$ electron to the 2π orbital.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{14}\text{N}^{16}\text{O}$ (continued)											
$\dots 4s^2 1\pi^4 2\pi \begin{Bmatrix} nd\lambda \\ np\lambda \end{Bmatrix}$										Narayana and Price's absorption Rydberg series converging to $c^3\Pi$ of NO^+ ; $v = 175220 - \begin{cases} R/(n+0.05)^2, & n = 3\dots 7. \\ R/(n-0.70)^2, & n = 3\dots 6. \end{cases}$ All bands diffuse. ^a Fragments of an additional series (181). Absorption cross sections $700 - 180 \text{ \AA}$ ($143000 - 556000 \text{ cm}^{-1}$) (164)(168).	(157)* (181)
$\dots 5s 1\pi^4 2\pi np\lambda$										Tanaka's absorption Rydberg series converging to $A^1\Pi(v=0)$ and $b^3\Pi(v=0)$ of NO^+ ; $v \approx \begin{cases} 147805 - R/(n-0.78)^2; & \gamma \text{ series}, n = 3\dots 11. \\ 133570 - R/(n-0.70)^2; & \beta \text{ series}, n = 3\dots 15. \end{cases}$ Also fragments of weak series with $v'=1$.	(5)(51)* (126)
$\dots 1\pi^3 2\pi ns\sigma$										Rydberg series converging to $a^3\Sigma^+$, $w^3\Delta$, $b^3\Sigma^-$, $A^1\Sigma^-$, $w^1\Delta$ of NO^+ . Only the first two or three members of each absorption series have been identified; long upper state progressions. Tables of absorption features $950 - 650 \text{ \AA}$ ($105000 - 154000 \text{ cm}^{-1}$) (5)(51)* (97)*. Absorption coefficients, photoionization and photodissociation yields (85)(97)(103)(146)(176). The band structure of the absorption spectrum from 80000 to 105000 cm^{-1} has not yet been analyzed. Absorption coefficients, photoionization efficiency curves (58)(85)(103); the data of (103) are conveniently plotted in Figure 6 of (165) and Figure 4 of (153). Autoionization processes have been studied by photoelectron spectroscopy (137)(165)(199); partial cross-sections for the formation of vibrationally excited NO^+ (153). Atlas of the absorption spectrum $1420 - 1250 \text{ \AA}$ ($70400 - 80000 \text{ cm}^{-1}$) (192); for a photographic reproduction of the spectrum at longer wavelengths ($1920 - 1400 \text{ \AA}$) see (42). A useful quantitative low-resolution plot of the absorption from 2300 to 1100 \AA may be found in Figure 2.1 of (192a), adapted from (13). Absorption coefficients, photoionization efficiency curves (17)(103)(166) and (195) whose supersonic molecular beam technique made it possible to resolve the autoionization structure superimposed on the first four vibrational steps due to direct ionization.	(126)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^{16}\text{O}$ (continued)										
		Rydberg series converging to $v=0\dots 4$ of $X^1\Sigma^+$ of NO^+ and fragments of series with $v'=5$:								
nf series		n = 4...15. Sharp rotational structure.						$nf \leftarrow X$		(192)*(204)*
nd δ series	{	Joining on to $F^2\Delta(n=3)$, $N^2\Delta(n=4)$, $U^2\Delta(n=5)$, and incompletely observed to $n=8$. Perturbations by stable and unstable states.						$nd\delta \leftarrow X$		(192)*(192a) (204)*
np π, σ series		Joining on to $C^2\Pi, D^2\Sigma^+(n=3)$, $K^2\Pi, M^2\Sigma^+(n=4)$, $Q^2\Pi, R^2\Sigma^+(n=5)$, and $W^2\Pi, Y^2\Sigma^+(n=6)$; bands of varying diffuseness have been observed to $n=11$. The influence of the unstable $A'^2\Sigma^+$ state is briefly discussed in (204).						$np\pi, \sigma \leftarrow X$		(192)*(192a) (204)*
ns σ series		Joining on to $A^2\Sigma^+(n=3)$, $E^2\Sigma^+(n=4)$, $S^2\Sigma^+(n=5)$, $T^2\Sigma^+(n=6)$, $Z^2\Sigma^+(n=7)$. The B_e values decrease from 1.997 ($n=3$) to 1.713 for the highest observed state ($n=11$) as a consequence of $ns\sigma \sim (n-1)d\sigma$ interactions, see ^f on p. 471. Sharp rotational structure.						$ns\sigma \leftarrow X$		(192)*(192a) (204)*
		Several unassigned non-Rydberg levels, mixed with Rydberg levels, near the dissociation limit $^2D + ^3P$ at 71627 cm^{-1} .								(74)(192)*
6f 71427		2376	H	16.2				$6f \leftarrow X,$	71543 71662.6	H (91)(192)*
6d δ (71342)		(2397)	H	(23)	[1.86]	$v=1,2,3$ diffuse.		$6d\delta \leftarrow X, v$	71467 71586 ^c	Z (91)(192)* (204)
$Z^2\Sigma^+ 7s\sigma$ 71224		2377	H	16.4	[1.938]			$Z \leftarrow X, v$	71340 71460 ^c	Z (91)(192)*

NO: ^aPhotoionization yields (NO^+ , N^+ , O^+) in the region of these Rydberg series (175).

^bThe Rydberg formulae do not accurately reproduce the observed bands owing to the slow variation of the quantum defect with n .

^cThese band origins refer to $N'=0$ (non-existent for $\Lambda \neq 0$) in the excited state and to the hypothetical level $J''=0$ of the $X^2\Pi_{3/2}$ ground state, in accordance with definitions adopted in these tables. The corresponding numbers for the $X^2\Pi_{3/2}$ component are obtained by subtracting 119.7 cm $^{-1}$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^{16}\text{O}$ (continued)										
Y $2\Sigma^+$ 6p δ	70614	2370	15.0	[2.11]	v=1,2,3 diffuse			Y \leftarrow X, V	70728 70847 ^a	(74)(91) (192)*
W 2Π 6p π	70512	2375	15.6		v=0 perturbed by non-Rydberg level; v=1,2,3 very diffuse.			W \leftarrow X,	70627 70747	(74)(91) (192)*
	5f 70079	2377	H	16.5	[1.988] ^b			5f \leftarrow X,	70195 ^c 70315 ^c	(91)(119) (192)*
U 2Δ 5d δ (69977)		2371		16.4	{ Partial rot. analyses for v=0,1 ($^{15}\text{N}^{18}\text{O}$). Perturbations by non-Rydberg levels. v=2,3,4 diffuse to varying degrees.			U \leftarrow X,	(70090) (70210)	(91)(192)* (204)
T $2\Sigma^+$ 6s δ (69728)		2372		15.7	v=0 coincides with I(v=6) and E(v=4), strong perturbation. $B_1 = 1.92$.			T \leftarrow X, V	(69841) (69961)	(91)(192)*
R $2\Sigma^+$ 5p δ (68598)					[2.04] ^d v=1,2 diffuse			R \leftarrow X, V	68710.9 68830.7 ^a	(74)(192)*
Q 2Π 5p π		v=0,1 mixed with non-Rydberg levels, v=2,3,4 diffuse.						Q \leftarrow X,	68526 68646	(74)(192)*
O' 2Π π (67762) ^e		(2371)	(16)	[2.022] ^f				O, O' \rightarrow D,	14702.2 14697.9	(64)(121)*
O $2\Sigma^+$ 4d δ 6 (67757)				[1.990] ^f				O, O' \rightarrow C,	15623 15619	(64)(121)*
								O, O' \leftarrow X,	67874.8 67870.5 ^a 67994.5 ^a 67990.3 ^a	(91)(121)*
	4f 67596	2381	H	18.5	[1.988] ^b		[1.065 ₇]	4f \leftarrow X,	67713 67833 ^c	(91)(119)*
N 2Δ 4d δ	67374	2375 ^g		15 ^g	1.969 ^g	0.026 ^g		N \rightarrow C, ^h	15238 ^g	(64)(135)*
								N \leftrightarrow X, V	67489 67609 ^g	(74)(76)* (88)*
S $2\Sigma^+$ 5s δ	66900	2378	Z	16.5	1.980	0.020		S \leftarrow X, V	67016 67136 ^a	(52)(74)(90)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^{16}\text{O}$ (continued)										
M $2\Sigma^+$ 4p σ 64437		2352	Z 19.5	2.022 ⁱ	0.018			M \leftarrow X, V 64540 64660 ^a	Z	(36)(52)(74) (90)* (192)*
K 2Π 4p π		v=0...3 observed.		[1.895] ^{jk}				K \leftarrow X, V 64167 64287 ^{al}	Z	(52)(74) (90)*
I $2\Sigma^+$ (63500)		{ Five levels (v=4...8?) have been observed for various isotopes in the region 67800 - 72000 cm^{-1} . Erratic behaviour with regard to diffuseness and isotope shifts on account of interactions with the unstable A' $2\Sigma^+$ state and with np σ Rydberg states. See also (160).						I \leftarrow X, R		(74)(204)

NO: ^aSee ^c on p. 469.

^bB value of the NO⁺ core. For details of the analysis and derived core parameters (polarizability, quadrupole moment) see (119).

^cEnergy of the Δ (or $\mathcal{L}=2$) component relative to the hypothetical level $J''=0$, calculated using results from the analysis of the $^{14}\text{N}^{18}\text{O}$ spectrum; see (119).

^dThe interaction between $R^2\Sigma^+(v=0)$, $I^2\Sigma^+(v=5?)$, and the continuous A' $2\Sigma^+$ state has been observed in the spectra of four isotopes; see Figure 2.5 of (192a).

^eA slight mixing of the ground state into the nd π components is responsible for the larger than expected spin-orbit coupling in H' (A = +0.96, ξ = +0.92) and O' (A = +0.36, ξ = +0.34); see (129), also (57)(121)(143).

^fStrong l -uncoupling, $\eta(v=0) = 1.92$ and 1.88 for 3d and 4d, resp. (143). The magnitude of η was interpreted in terms of s \sim d mixing (129); the interaction matrix elements are 910 (4s σ ~3d σ) and 430 cm^{-1} (5s σ ~4d σ). The non-negligible

spin-orbit coupling in nd π (see ^e) gives rise to small perturbations between e levels of the 2Π F₁ and F₂ components (56)(57)(121)(143). Additional perturbations in H,H' by Rydberg and non-Rydberg levels (143). For H,H' (v=3) only Π^- has been observed. The Π^+ and Σ^+ components of O,O' (v=0) are weakly predissociated for all N, Π^- above N=16 (121).
^gApproximate deperturbed constants, see ^p on p. 473; v=3 at 74580 cm^{-1} is very diffuse (204).

^hThe N \rightarrow C 0-0 band is strongly mixed with B' \rightarrow C 7-0; see ^q on p. 473.

ⁱHeterogeneous perturbations by levels of B 2Π (112). Levels having v \geq 1 are diffuse to varying degrees.

^jA small perturbation by L 2Π (v=2?) affects the first few rotational levels in v=0; higher vibrational levels (v = 1,2,3) are strongly mixed with non-Rydberg states (B 2Π and L 2Π).

^k Λ -type doubling, $\Delta v_{fe}(F_1) = +0.034 N(N+1)$.

^lDeperturbed.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^{16}\text{O}$ (continued)										
G $^2\Sigma^-$	62913.0	1085.54	Z	11.083 ^a	1.2523 ^b	0.0204	1.3427	G \leftarrow X, ^c R	62384.7 ^d 62504.4 ^d Z	(69)* (192)* (204)
L $^2\Pi_i$	(62500) ^e	Fragments of several levels (vibr. numbering not established) in perturbations with levels of B, C, K. Constants comparable to B $^2\Pi$.						L \leftarrow X		(74)(90)*
H' $^2\Pi$	π 62485.4 ^f	2371.3	Z	16.17	2.015 ^g	0.021	1.058 ₅	H, H' \rightarrow D, ^h	9426.0 9414.2	(55)(64)*
H $^2\Sigma^+$	$3d$ 62473.4	[2339.4]	Z		2.003 ^g	0.018	1.061 ₇	H, H' \rightarrow C, ^h	10348 10336	(55)(64) (121)*
								H, H' \rightarrow A, ^h	18518.2 18506.4	(55)(64)*
									62598.6	
								H, H' \leftarrow X, ⁱ	62586.8 62718.4 ^d Z	(56)(91) (143)*
									62706.6 ^d Z	
F $^2\Delta$	$3d\delta$ 61800	2394 ^j		20 ^j	1.982 ^j	0.023 ^j	1.067	F \rightarrow C, ^{kh}	9670 ^j	(64)(135)*
								F \leftrightarrow X, ⁱ V	61924 ^j 62044 ^j	(52)(74) (76)* (88)*
E $^2\Sigma^+$	$4s\sigma$ 60628.8	2375.3	Z	16.4 ₃	1.9863 ^l	0.0182	5.6	E \rightarrow D, ^{hm}	7571.5	(9)(45)
								E \rightarrow A, ^h		
								"6000 \AA " b.	16663.63 Z	(9)* (143)*
								E \leftarrow X, ⁿ V	60744.1 60863.8 ^d Z	(11)(26) (42)* (74)
B' $^2\Delta_i$	60364.2 ^o	1217.4 ^p		15.61 ^p	1.332 ^p	0.021 ^p	1.302	B' \rightarrow C, ^q		(64)(135)*
								B' \rightarrow B, ⁿ V	14508.6 14538.7	(12)(14)(31) (64)
								B' \leftrightarrow X, ^{sn} R	59900.7	(10)(12)(15)
								β' bands	60020.4 ^d Z	(16)(26)(22)* (74)(76)*(88)*
D $^2\Sigma^+$	$3p\sigma$ 53084.7	2323.90	Z	22.885 ^t	2.0026 ^u	0.02175	[5.8]	D ^v \rightarrow A, ^h	9092.17 Z	(9)(64) (112)*(143)*
								"11000 \AA " b.		
								D ^v \leftrightarrow X, ^{nw} V	53172.7	(1)* (6)* (7) (12)(16)(24)
								ϵ bands	53292.4 ^d Z	(37)(42)* (90)(112)* (144)

NO: ^a $w_e y_e = -0.1439$. The levels $v=10, 11, 12$ are diffuse and lie above the limit $^2D + ^3P$; $v=13$ not observed. See also ^bSmall perturbations in isotope spectra. (160).
^cAbsorption in rare gas matrices (101)(197), in high pressure argon (190).
^dSee ^c on p. 469.
^e $A \approx -80$.
^fSee ^e on p. 471.
^gSee ^f on p. 471.
^hFor experimental and theoretical f values see (122)(140) and (138), respectively.
ⁱAlso observed by non-resonant multiphoton ionization spectroscopy (189).
^jApproximate deperturbed constants; see ^P.
^kLines of the perturbed $F \rightarrow C$ 1-1 band are prominent in the NO laser spectrum (179); see ^{P, q}.
^l $v=3, 4$ somewhat diffuse, $v=5$ sharp. Emission observed from $v \leq 2$; (64) reports an abrupt breaking-off in the $E \rightarrow A$ 2-2 band for an upper state energy of 68100 cm^{-1} .
^m $E \rightarrow C$ not observed, in agreement with theoretical predictions (138) regarding the dipole transition strengths of $E \rightarrow C$ and $E \rightarrow D$.
ⁿFor references to Franck-Condon factor calculations see the review by (99).
^o $A_0 = -2.2, A_1 = -2.4, \dots, A_9 = -4.9$ (88).
^pDeperturbed constants; $B'^2\Delta$ interacts strongly with $F^2\Delta$ (matrix element $H_e \approx 450 \text{ cm}^{-1}$) and $N^2\Delta$ ($H_e \approx 400$) (84)(88); see also ^s. Perturbations by $B^2\Pi$ are unobservably small because of unfavourable Franck-Condon factors (191b).

^qFragments of two bands, 4-1 at 9800 cm^{-1} and 7-0 at 15300 cm^{-1} , both appearing on account of configuration interaction, in the upper state with $F^2\Delta$ and $N^2\Delta$, respectively, in the lower state with $B^2\Pi$. Lines of the 4-1 band, together with $F \rightarrow C$ 1-1, are seen in the NO laser spectrum (65)(89)(162)(179).
^rLifetime $\tau(v=1) = 75 \text{ ns}$ (174).
^sAn experimentally deperturbed spectrum of $B'-X$ is observed in matrix absorption (101)(116)(197). A gradual deperturbation in the gas phase is induced by increasingly high foreign gas pressures (190).
^t $w_e y_e = +0.75, w_e z_e = -0.22$, from $v \leq 4$ (36), not including $v=5$ and 6 (90). The vibrational constants clearly differ from those of other Rydberg $^2\Sigma$ states or of the NO^+ ground state. It has been suggested [see e.g. (143), also (160)] that there is an avoided crossing of the potential curves of $D^2\Sigma^+$ and $A'^2\Sigma^+$ (unstable, arising from $^4S + ^3P$).
^uFrom (36). Heterogeneous perturbations by $B^2\Pi$; for details see (112). According to (64) the rotational structure of $D \rightarrow A$ 1-1, 2-2, 3-3 breaks off abruptly at D state energies of 59270 cm^{-1} in $v=1, 2$ and 60100 cm^{-1} in $v=3$.
^vLifetimes $\tau(v=0) = 18.4 \text{ ns}$ (106), 19.0 ns (183), 25.7 ns (174); $\tau(v=1) = 26.4 \text{ ns}$ (174).
^w $f_{00} = 0.0025, f_{10} = 0.0046, f_{20} = 0.0033$; from integrated absorption intensities (43). See also (62)(124).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{14}\text{N}^{16}\text{O}$ (continued)										
C $^2\Pi_r$ 3p π 52126 ^a		2395 ^b	15 ^b	2.000 ^{bc}	0.030 ^b		1.062	C ^c →A, ^d	8172	(45)(117)* (187)*
								C ^c ↔X, ^{ef} v	52251	(1)* (3)(4)*
								δ bands	52371	(6)(30)(42)* (90)(117)* (144)
									10395	
									10375	
b ($^4\Sigma^-$) (48680)		1206 ^g	H 15					b→a, v	10350 ^g H	(18)*(19)*
									10323	
									10300	
									10272	
B $^2\Pi_r$	45942.6 ^h	1039.8 ⁱ	Z	8.3 ₂ ^j	1.152 ⁱ	0.012		B ^m ↔X, ^{nf} R	45392.1 ^o Z	(1)*(2)*(6)* (3)(15)(18)*
	45913.6	1037.2 ⁱ	Z	7.7 ₀ ^k	1.092 ^{il}	0.012	4.9	β bands	45481.7 ^o Z	(24)(31)(37) (42)*(73)* (52)(90)(127)
A $^2\Sigma^+$ 3s σ	43965.7	2374.31	Z	16.106 ^p	1.9965 ^{qrs}	0.01915 ^q	5.4	A ^t ↔X, ^{uvf} v	44080.5	(1)* (3)(8)
								γ bands	44200.2 ^w Z	(24)(37)(46) (127)
a ($^4\Pi_1$) (38440)		1017	H 11					(a→X) ^x		(48)(66)
								M bands	(38000)	

NO: ^a $A_0 = + 3.0 \text{ cm}^{-1}$ (104).

^bApproximate deperturbed constants; strong interaction with B $^2\Pi$, see ⁱ. Λ -type doubling, $\Delta v_{fe}(F_1) = +0.016N(N+1)$.

^cWeak predissociation in $v=0$ above $N=3$ or 4 [see (179)(187) and ^a on p. 467]. The predissociation is assumed to occur via the continuum of the a $^4\Pi$ state and causes a reduction of the measured lifetimes in $v=0$ from 20 ns for $N \leq 4$ to 3 ns for $N \geq 4$ (183); $\tau(v=1) \leq 0.3$ ns. No emission has been observed from levels having $v \geq 1$.

^dSee ^h on p. 473.

^e $f_{00} = 0.0023$ (43)(177), higher value in (124); $f_{10} = 0.0058$, $f_{20} = 0.0027$ (43). See also (62).

^fSee ⁿ on p. 473. RKR Franck-Condon factors for the β bands (111)(128), for the γ bands (111)(134).

^gA different vibrational numbering was suggested by (75).

^h $A_v = + 31.32 + 1.152(v+\frac{1}{2}) + 0.0448(v+\frac{1}{2})^2$. The expression represents the data of (127) for the first seven levels.

A_v increases to +77 for $v=25$; see (90).

NO (continued):

ⁱEffective constants for $v \leq 5$ (73). The re-evaluation of the constants by (127), based on new measurements of the β bands and using a modified Hill-Van Vleck expression, gave $G(v) = 1037.45(v+\frac{1}{2}) - 7.472(v+\frac{1}{2})^2 + 0.0725_3(v+\frac{1}{2})^3$,

$$B_v = 1.1250 - 0.01348(v+\frac{1}{2}) + 0.00012_5(v+\frac{1}{2})^2.$$

The highest level observed in emission is $v'=7$ [mixed with $C(v=0)$] (49)(117); vibrational levels as high as $v'=29$ have been identified in the absorption spectrum (74). They are strongly perturbed by interaction with the Rydberg states $C^2\Pi$ (matrix element $H_e \approx 1200 \text{ cm}^{-1}$) and $K^2\Pi$ ($H_e \approx 800$); see (42)(84). A complete deperturbation, taking also into account the interaction with $L^2\Pi$, was attempted by (136); more recent results by Galusser and Dressler ($\omega_e = 1025.0$, $\omega_e x_e = 4.52$, $\omega_e y_e = -0.0846$) are quoted by (185) who observed the deperturbed spectrum of $B^2\Pi$ in matrix absorption (101)(116). A similar deperturbation is induced by high pressure foreign gases (190). Heterogeneous interactions with levels of $D^2\Sigma^+$ and $M^2\Sigma^+$ are discussed by (112).

$$^j \omega_e y_e = + 0.17.$$

$$^k \omega_e y_e = + 0.10.$$

$$^l \Lambda\text{-type doubling, } \Delta v_{fe}(v=0) = -0.0064(J+\frac{1}{2}) \text{ (64).}$$

^mRadiative lifetimes $\tau(v=0,1,4) = 1.9_9, 1.7_8, 1.6_5 \text{ } \mu\text{s}$, resp. (174). (68) give somewhat longer lifetimes.

ⁿ $f_{00} = 2.5 \times 10^{-8}$ (141); $f_{v,0}$ values increase to 4.6×10^{-5} for $v'=6$ (43)(141)(150). Above $v'=7$ the intensities are governed by the strong interactions with the $3p$ and $4p$ Rydberg states; see ⁱ. See also (59)(62)(70)(105).

^oReferring to the hypothetical $J=0$ levels in both upper and lower state.

$$^p \omega_e y_e = - 0.0465 \text{ (127).}$$

^qRotational constants re-evaluated from data in (36) and (127); the equilibrium constants of the latter appear unreliable.

^rSpin splitting constant $\gamma(v=3) = - 0.0027650$, $\mu_{ef}(v=3) = 1.10 \text{ D}$. These constants, as well as eqQ and magnetic hf constants, have been recalculated by (194) from the optical-rf double resonance experiment of (172); see also (152)(191). Hanle effect (139)(151a)(159).

^sAccording to (8)(41) the intensity of the emission bands drops sharply at $N' = 74, 64, 52, 38$ in $v' = 0, 1, 2, 3$, respectively; bands with $v' \geq 4$ have not been observed in emission.

^tRadiative lifetimes $\tau(v=0) = 215 \text{ ns}$, $\tau(v=1) = 203 \text{ ns}$, $\tau(v=2) = 174 \text{ ns}$ (206); good agreement with (174) except for $v=2$ where these authors find $\tau = 195 \text{ ns}$. See also (87)(159)(183).

^u $f_{00} = 0.00038$, $f_{10} = 0.00081$, $f_{20} = 0.00069$, $f_{30} = 0.00030$; weighted average values from (38)(43)(132)(150)(151). Variation of transition moment with r (70)(83)(87)(93)(105)(111)(149); see also (144).

^vAlso observed in two-photon excitation (173)(186)(206) and magnetic rotation spectra (100). $^{15}\text{N}^{16}\text{O}$ band head measurements (125).

^wSee ^c on p. 469.

^xAssignment uncertain, only observed in rare gas matrices. Predicted lifetime 0.1 s (115). See also (170).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
¹⁴ N ¹⁶ O (continued)										
X $^2\Pi_r$	119.82 ^a 0	1904.04 ₀ Z 1904.20 ₄ Z	14.100 ^b 14.075 ^b	[1.72016] ^c [1.67195] ^{cd}	0.0182 0.0171	[10.2 ₃] ^c [0.5 ₄] ^c	1.15077	$\frac{3}{2} \leftarrow \frac{1}{2},^e$	119.73 ^f Z	(148)
<p>NO: ^a$A_v = +123.26 - 0.1906(v+\frac{1}{2}) - 0.0108(v+\frac{1}{2})^2$; from the analysis of β and γ bands having $v'' \leq 16$ (127). Much more precise constants for $v=0$ and 1 ($A_{\text{eff}} = 123.1393$ and 122.8935, respectively) and their J dependence have been determined from measurements on the vibration-rotation fundamental and on the pure rotation spectrum (205)(209). See also (148)(156).</p> <p>^b$w_e y_e = +0.011_0 (^2\Pi_{3/2})$ and $+0.007_7 (^2\Pi_{1/2})$; these are effective vibrational constants obtained from rotation-vibration spectra (67)(77). (205)(209) have accurately evaluated $\Delta G(\frac{1}{2}) = 1875.972$; see ^a. (127), see ^a, give the following expression, valid for $v \leq 16$: $G(v) = 1904.40_5(v+\frac{1}{2}) - 14.187_0(v+\frac{1}{2})^2 + 0.0240_0(v+\frac{1}{2})^3 - 0.00093(v+\frac{1}{2})^4$. The vibrational levels have been observed to $v=23$ (18).</p> <p>^cEffective rotational constants from rotation (29)(44)(86) and rotation-vibration spectra (191a)(205). Precise B and D values for $v=0$ and 1 have been calculated by (209), see ^a: $B_0 = 1.69611_5$, $B_1 = 1.67854_4$; $D_0 = 5.3_4 \times 10^{-6}$, $D_1 = 5.3_7 \times 10^{-6}$; good agreement with (205). (127), see ^a, give the following expression for $v \leq 16$: $B_v = 1.7042_7 - 0.01728(v+\frac{1}{2}) - 0.000037(v+\frac{1}{2})^2$.</p>								Rotation-vibration sp. ⁱ		
								$4 \rightarrow 2$		(63)
								$4 \leftarrow 0$		(77)(78)
								$3 \rightarrow 1$		(63)
								$3 \leftarrow 0,^{gh}$		(23)(54)(71) (72)(77)
								$2 \leftarrow 1$		(208)
								$2 \leftrightarrow 0,^{ghi}$		(23)(63)(72) (77)
								$1 \leftrightarrow 0,^{ghijklmn}$		(32)(34)(61) (67)(113) (205)(209)
								Rotation sp. ^o		(29)(33)(44) (86)(148)
								Raman sp. ^p		(120)(133)
								EPR sp.		(82)(145) (193)
								Hyperfine Λ -doubl. sp. ^q		(131)(154) (200)

^gMagnetic rotation (50)(81)(107)(114)(161).^hIntegrated band intensities, dipole moment function (92) (142)(163)(167); (184)(198).ⁱ $2-0$ b. of $^{15}\text{N}^{18}\text{O}$ (96), $1-0$ b. of $^{15}\text{N}^{16,18}\text{O}$ (39)(96)(113).

NO (continued):

- ^j Λ -doubling, nuclear hfs, and Zeeman splittings (147)(158).
² $\Pi_{3/2}$ laser magnetic resonance spectra (171)(191a).
^kLaser Stark spectrum (188); $\mu_{el}(^2\Pi_{1/2}, v=0) = 0.157_4$ D (see also ^q), $\mu_{el}(^2\Pi_{1/2}, v=1) = 0.1416$ D. For ² $\Pi_{3/2}$ the difference $\mu_{el}(v=1) - \mu_{el}(v=0) = -0.01735$ D was determined.
^lFrom pressure-broadened linewidths (196) derive a value of 2.4×10^{-26} esu cm² for the quadrupole moment of NO. Earlier results are reviewed in this paper.

- (1) Leifson, ApJ 63, 73 (1926).
- (2) Jenkins, Barton, Mulliken, PR 30, 150 (1927).
- (3) Schmid, ZP 40, 428 (1928); 64, 84 (1930).
- (4) Schmid, ZP 64, 279 (1930).
- (4a) Rasetti, ZP 66, 646 (1930).
- (5) Tanaka, Sci. Pap. IPCR (Tokyo) 32, 456 (1942).
- (6) Gaydon, PPS 56, 95, 160 (1944).
- (7) Gerö, Schmid, von Szily, Physica 11, 144 (1944).
- (8) Gerö, Schmid, PPS 60, 533 (1948).
- (9) Feast, CJR A 28, 488 (1950).
- (10) Baer, Miescher, HPA 24, 331 (1951).
- (11) Tanaka, Seya, Mori, JCP 19, 979 (1951).
- (12) Baer, Miescher, Nature 169, 581 (1952); HPA 26, 91 (1953).
- (13) Marmo, JOSA 43, 1186 (1953).
- (14) Ogawa, SL 2, 87 (1953).
- (15) Sutcliffe, Walsh, PPS A 66, 209 (1953).
- (16) Tanaka, JCP 21, 788 (1953).
- (17) Watanabe, Marmo, Inn, PR 91, 1155 (1953); Watanabe, JCP 22, 1564 (1954).
- (18) Brook, Kaplan, PR 96, 1540 (1954).

- ^mAbsorption of CO laser radiation by NO (202)(203)(207).
ⁿ $\Delta v=1$ sequence in emission (201). Several laser lines have been observed in the P branches of the 6-5, ..., 11-10 bands (83a).
^oZeeman effect (21), Stark effect (40), both in ² $\Pi_{1/2}$.
^pSee also references in ^e.
^q $\mu_{el} = 0.15872$ D from Stark effect in ² $\Pi_{1/2}, v=0, J=\frac{1}{2}$ (131); eqQ and other hf coupling constants (154)(200). See also (152) (191).

- (19) Ogawa, SL 3, 39 (1954).
- (20) Tanaka, JCP 22, 2045 (1954).
- (21) Mizushima, Cox, Gordy, PR 98, 1034 (1955).
- (22) Miescher, CJP 33, 355 (1955); HPA 29, 401 (1956).
- (23) Nichols, Hause, Noble, JCP 23, 57 (1955).
- (24) Ogawa, SL 3, 90 (1955).
- (25) Sun, Weissler, JCP 23, 1372 (1955).
- (26) Ueda, SL 3, 143 (1955).
- (27) Walker, Weissler, JCP 23, 1962 (1955).
- (28) Granier, Astoin, CR 242, 1431 (1956).
- (29) Gallagher, Johnson, PR 103, 1727 (1956).
- (30) Herzberg, Lagerqvist, Miescher, CJP 34, 622 (1956).
- (31) Ogawa, Shimauchi, SL 5, 147 (1956).
- (32) Shaw, JCP 24, 399 (1956).
- (33) Palik, Rao, JCP 25, 1174 (1956).
- (34) Thompson, Green, SA 8, 129 (1956).
- (35) Astoin, JRCNRS No. 38, 1 (1957).
- (36) Barrow, Miescher, PPS A 70, 219 (1957).
- (37) Deézi, Mátrai, APH 7, 111 (1957).
- (38) Weber, Penner, JCP 26, 860 (1957).
- (39) Fletcher, Begun, JCP 27, 579 (1957).

- NO: (40) Burrus, Graybeal, PR 109, 1553 (1958).
 (41) Deézsi, APH 9, 125 (1958).
 (42) Lagerqvist, Miescher, HPA 31, 221 (1958).
 (43) Bethke, JCP 31, 662 (1959).
 (44) Favero, Mirri, Gordy, PR 114, 1534 (1959).
 (45) Heath, Los Alamos Report LA-2335 (1959).
 (46) Koczkás, APH 10, 117 (1959).
 (47) Maryott, Kryder, JCP 31, 617 (1959).
 (48) Broida, Peyron, JCP 32, 1068 (1960).
 (49) Deézsi, APH 11, 155 (1960).
 (50) Mann, Hause, JCP 33, 1117 (1960).
 (51) Huber, HPA 34, 929 (1961).
 (52) Lagerqvist, Miescher, CJP 40, 352 (1962).
 (53) Miescher, JQSRT 2, 421 (1962).
 (54) Arcas, Haeusler, Joffrin, Meyer, van Thanh, Barchewitz, AO 2, 909 (1963).
 (55) Huber, Huber, Miescher, PL 3, 315 (1963).
 (56) Huber, Miescher, HPA 36, 257 (1963).
 (57) Kovács, HPA 36, 699 (1963).
 (58) Nicholson, JCP 39, 954 (1963).
 (59) Antropov, Dronov, Sobolev, OS(Engl. Transl.) 17, 355 (1964).
 (60) Callear, Smith, DFS 37, 96 (1964).
 (61) James, JCP 40, 762 (1964).
 (62) Ory, JCP 40, 562 (1964).
 (63) Horn, Dickey, JCP 41, 1614 (1964).
 (64) Huber, HPA 37, 329 (1964).
 (65) Huber, PL 12, 102 (1964).
 (66) Frosch, Robinson, JCP 41, 367 (1964).
 (67) James, Thibault, JCP 41, 2806 (1964).
 (68) Jeunehomme, Duncan, JCP 41, 1692 (1964).
 (69) Lofthus, Miescher, CJP 42, 848 (1964).
 (70) Marr, PPS 83, 293 (1964).
 (71) Meyer, Haeusler, van Thanh, Barchewitz, JP(Paris) 25, 337 (1964).
 (72) Olman, McNelis, Hause, JMS 14, 62 (1964); 21, 111 (1966) (erratum).
 (73) Callear, Smith, TFS 61, 1303 (1965).
 (74) Dressler, Miescher, ApJ 141, 1266 (1965).
 (75) Gilmore, JQSRT 5, 369 (1965).
 (76) Jungen, Miescher, ApJ 142, 1660 (1965).
 (77) Meyer, Haeusler, Barchewitz, JP(Paris) 26, 799 (1965).
 (78) Meyer, Haeusler, CR 260, 4182 (1965).
 (79) Abels, Shaw, JMS 20, 11 (1966).
 (80) Alamichel, JP(Paris) 27, 345 (1966).
 (81) Aubel, Hause, JCP 44, 2659 (1966).
 (82) Brown, Radford, PR 147, 6 (1966).
 (83) Callear, Pilling, Smith, TFS 62, 2997 (1966).
 (83a) Deutsch, APL 2, 295 (1966).
 (84) Felenbok, Lefebvre-Brion, CJP 44, 1677 (1966).
 (85) Reese, Rosenstock, JCP 44, 2007 (1966).
 (86) Hall, Dowling, JCP 45, 1899 (1966).
 (87) Jeunehomme, JCP 45, 4433 (1966).
 (88) Jungen, CJP 44, 3197 (1966).
 (89) Jungen, Miescher, Suter, PL 21, 36 (1966).
 (90) Lagerqvist, Miescher, CJP 44, 1525 (1966).
 (91) Miescher, JMS 20, 130 (1966).
 (92) Schurin, Ellis, JCP 45, 2528 (1966).
 (93) Antropov, Kolesnikov, Ostrovskaya, Sobolev, OS (Engl. Transl.) 22, 109 (1967).
 (94) Crosley, Zare, PRL 18, 942 (1967). [Erroneous, s.(139)]
 (95) Feinberg, Camal, JQSRT 7, 581 (1967).
 (96) Griggs, Rao, Jones, Potter, JMS 22, 383 (1967).
 (97) Metzger, Cook, Ogawa, CJP 45, 203 (1967).

- NO: (98) Oppenheim, Yair Aviv, Goldman, AO 6, 1305 (1967).
 (99) Ortenberg, Antropov, SPU 2, 717 (1967).
 (100) Robinson, JCP 46, 4525 (1967); 50, 5018 (1969).
 (101) Roncin, Damany, Romand, JMS 22, 154 (1967).
 (102) Varanasi, Penner, JQSRT 7, 279 (1967).
 (103) Watanabe, Matsunaga, Sakai, AO 6, 391 (1967).
 (104) Ackermann, Miescher, CPL 2, 351 (1968).
 (105) Antropov, Proc. (Trudy) P.N. Lebedev Phys. Inst. 35, 1 (1966) [Engl. Transl. Consultants Bureau, New York (1968)].
 (106) Hesser, JCP 48, 2518 (1968).
 (107) Buckingham, Segal, JCP 49, 1964 (1968).
 (108) Callear, Pilling, Smith, TFS 64, 2296 (1968).
 (109) Chardon, Théobald, CR B 266, 602 (1968).
 (110) Crosley, Zare, JCP 49, 4231 (1968). [Erroneous, s.
 (111) Jain, Sahni, TFS 64, 3169 (1968). | (139)]
 (112) Jungen, Miescher, CJP 46, 987 (1968).
 (113) Keck, Hause, JMS 26, 163 (1968).
 (114) Keck, Hause, JCP 49, 3458 (1968).
 (115) Lefebvre-Brion, Guérin, JCP 49, 1446 (1968).
 (116) Roncin, JMS 26, 105 (1968).
 (117) Ackermann, Miescher, JMS 31, 400 (1969).
 (118) Fast, Welsh, Lepard, CJP 47, 2879 (1969).
 (119) Jungen, Miescher, CJP 47, 1769 (1969).
 (120) Renschler, Hunt, McCubbin, Polo, JMS 32, 347 (1969).
 (121) Suter, CJP 47, 881 (1969).
 (122) Wray, JQSRT 2, 255 (1969).
 (123) Callear, Pilling, TFS 66, 1618 (1970).
 (124) Callear, Pilling, TFS 66, 1886 (1970).
 (125) Cisak, Danielak, Rytel, APP A 37, 67 (1970).
 (126) Edqvist, Lindholm, Selin, Sjögren, Åsbrink, AF 40, 439 (1970).
 (127) Engleman, Rouse, Peek, Baiamonte, Los Alamos Sci. Lab. Report LA-4364 (1970); Engleman, Rouse, JMS 37, 240
 (128) Generosa, Harris, JCP 53, 3147 (1970). | (1971).
 (129) Jungen, JCP 53, 4168 (1970).
 (130) Lepard, CJP 48, 1664 (1970).
 (131) Neumann, ApJ 161, 779 (1970).
 (132) Pery-Thorne, Banfield, JP B 3, 1011 (1970).
 (133) Shotton, Jones, CJP 48, 632 (1970).
 (134) Spindler, Isaacson, Wentink, JQSRT 10, 621 (1970).
 (135) Ackermann, CJP 49, 76 (1971).
 (136) Bartholdi, Leoni, Dressler, ZAMP 22, 797 (1971).
 (137) Collin, Delwiche, Natalis, IJMSIP 7, 19 (1971).
 (138) Gallusser, Dressler, ZAMP 22, 792 (1971).
 (139) German, Zare, Crosley, JCP 54, 4039 (1971).
 (140) Groth, Kley, Schurath, JQSRT 11, 1475 (1971).
 (141) Hasson, Nicholls, JP B 4, 1769 (1971).
 (142) Michels, JQSRT 11, 1735 (1971).
 (143) Miescher, CJP 49, 2350 (1971).
 (144) Poland, Broida, JCP 54, 4515 (1971); JQSRT 11, 1863
 (145) Ashford, Jarke, Solomon, JCP 57, 3867 (1972). | (1971).
 (146) Bahr, Blake, Carver, Gardner, Kumar, JQSRT 12, 59 (1972).
 (147) Blum, Nill, Calawa, Harman, CPL 15, 144 (1972).
 (148) Brown, Cole, Honey, MP 23, 287 (1972).
 (149) Bubert, JCP 56, 1113 (1972).
 (150) Farmer, Hasson, Nicholls, JQSRT 12, 627, 635 (1972).
 (151) Hasson, Farmer, Nicholls, Anketell, JP B 5, 1248
 (151a) Gouédard, AP(Paris) 7, 159 (1972). | (1972).
 (152) Green, CPL 13, 552 (1972); 23, 115 (1973).
 (153) Kleimenov, Chizhov, Vilesov, OS(Engl. Transl.) 32, 371
 (154) Meerts, Dymanus, JMS 44, 320 (1972). | (1972).
 (155) - s. (192a)
 (156) Mizushima, Evenson, Wells, PR A 5, 2276 (1972).

- NO: (157) Narayana, Price, JP B 5, 1784 (1972).
 (158) Nill, Blum, Calawa, Harman, CPL 14, 234 (1972).
 (159) Weinstock, Zare, Melton, JCP 56, 3456 (1972).
 (160) Ben-Aryeh, JQSRT 13, 1441 (1973).
 (161) Blum, Nill, Strauss, JCP 58, 4968 (1973).
 (162) Broida, Miescher, JQE 2, 1029 (1973).
 (163) Chandraiah, Cho, JMS 47, 134 (1973).
 (164) Gardner, Lynch, Stewart, Watson, JP B 6, L262 (1973).
 (165) Gardner, Samson, JESRP 2, 153 (1973).
 (166) Killgoar, Leroy, Berkowitz, Chupka, JCP 58, 803 (1973).
 (167) Konkov, Vorontsov, OS(Engl. Transl.) 34, 595 (1973).
 (168) Lee, Carlson, Judge, Ogawa, JQSRT 13, 1023 (1973).
 (169) Mandelman, Carrington, Young, JCP 58, 84 (1973).
 (170) Zarur, Chiu, JCP 59, 82 (1973).
 (171) Zeiger, Blum, Nill, JCP 59, 3968 (1973).
 (172) Bergeman, Zare, JCP 61, 4500 (1974).
 (173) Bray, Hochstrasser, Wessel, CPL 27, 167 (1974).
 (174) Brzozowski, Elander, Erman, PS 2, 99 (1974).
 (175) Hertz, Jochims, Schenk, Sroka, CPL 29, 572 (1974).
 (176) Hertz, Jochims, Sroka, PL A 46, 365 (1974).
 (177) Mandelman, Carrington, JQSRT 14, 509 (1974).
 (178) Morioka, Nakamura, Ishiguro, Sasanuma, JCP 61, 1426 (1974).
 (179) Miescher, JMS 53, 302 (1974).
 (180) Miescher, in "Vacuum Ultraviolet Radiation Physics", p. 61 (ed. Koch, Haensel, Kunz). Pergamon-Vieweg, Braunschweig (1974).
 (181) Sasanuma, Morioka, Ishiguro, Nakamura, JCP 60, 327 (1974).
 (182) Takezawa, paper MG12, 29th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio (1974).
 (182a) Wight, Brion, JESRP 4, 313 (1974).
 (183) Benoist d'Azy, López-Delgado, Tramer, CP 2, 327 (1975).
 (184) Billingsley, JCP 62, 864; 63, 2267 (1975).
 (185) Boursey, Roncin, JMS 55, 31 (1975).
 (186) Bray, Hochstrasser, Sung, CPL 33, 1 (1975).
 (187) Dingle, Freedman, Gelernt, Jones, Smith, CP 8, 171 (1975).
 (188) Hoy, Johns, McKellar, CJP 53, 2029 (1975).
 (189) Johnson, Berman, Zakheim, JCP 62, 2500 (1975).
 (190) Miladi, Le Falher, Roncin, Damany, JMS 55, 81 (1975); Miladi, Thèse (U. de Paris-Sud, Centre d'Orsay, 1976).
 (191) Walch, Goddard, CPL 33, 18 (1975).
 (191a) Hakuta, Uehara, JMS 58, 316 (1975).
 (191b) Field, Gottscho, Miescher, JMS 58, 394 (1975).
 (192) Miescher, Alberti, JPCRD 5, 309 (1976).
 (192a) Miescher, Huber, International Review of Science, Physical Chemistry Series Two, Vol. 3, Spectroscopy (ed. Ramsay). Butterworths (1976).
 (193) Jarke, Ashford, Solomon, JCP 64, 3097 (1976).
 (194) Woods, Dixon, JCP 64, 5319 (1976).
 (195) Ng, Mahan, Lee, JCP 65, 1956 (1976).
 (196) Tejwani, Golden, Yeung, JCP 65, 5110 (1976).
 (197) Boursey, JMS 61, 11 (1976).
 (198) Billingsley, JMS 61, 53 (1976).
 (199) Caprace, Delwiche, Natalis, Collin, CP 13, 43 (1976).
 (200) Meerts, CP 14, 421 (1976).
 (201) Mantz, Shafer, Rao, AO 15, 599 (1976).
 (202) Richton, AO 15, 1686 (1976).
 (203) Hanson, Monat, Kruger, JQSRT 16, 705 (1976).
 (204) Miescher, CJP 54, 2074 (1976).
 (205) Valentin, Boissy, Cardinet, Henry, Chen, Rao, CR B 283, 233 (1976).
 (206) Zacharias, Halpern, Welge, CPL 43, 41 (1976).
 (207) Garside, Ballik, Elsherbiny, Shewchun, AO 16, 398 (1977).
 (208) Guerra, Sanchez, Javan, PRL 38, 482 (1977).
 (209) Johns, Reid, Lepard, JMS 65, 155 (1977).

NO⁺, NO⁺⁺ (continued from p.483):

- (12) Stair, Gauvin, in "Aurora and Airglow", p.365 (ed. McCormac). Reinhold, New York (1967).
- (13) Hesser, JCP 48, 2518 (1968).
- (14) Huber, CJP 46, 1691 (1968).
- (15) Nicholls, JP B 1, 1192 (1968).
- (16) Price, in "Molecular Spectroscopy", p.221 (ed. Hepple). The Institute of Petroleum, London (1968).
- (17) Samson, PL A 28, 391 (1968).
- (18) Sjögren, Szabo, AF 37, 551 (1968).
- (19) Jungen, Miescher, CJP 47, 1769 (1969).
- (20) Siegbahn, Nordling, Johansson, Hedman, Hedén, Hamrin, Gelius, Bergmark, Werme, Manne, Baer, "ESCA Applied to Free Molecules". North-Holland, Amsterdam (1969).
- (21) Edqvist, Lindholm, Selin, Sjögren, Åsbrink, AF 40, 439 (1970).
- (22) Jungen, Lefebvre-Brion, JMS 33, 520 (1970).
- (23) Wentink, Spindler, JQSRT 10, 609 (1970).
- (24) Aarts, de Heer, Physica 54, 609 (1971).
- (25) Edqvist, Åsbrink, Lindholm, ZN 26 a, 1407 (1971).
- (26) Lefebvre-Brion, CPL 2, 463 (1971).
- (27) Maier, Holland, JCP 54, 2693 (1971).
- (28) Moddeman, Carlson, Krause, Pullen, Bull, Schweitzer, JCP
- (29) Davis, Shirley, JCP 56, 669 (1972). | 55, 2317 (1971).
- (30) Mentall, Morgan, JCP 56, 2271 (1972).
- (31) Stone, Zipf, JCP 56, 2870 (1972).
- (32) Thulstrup, Öhrn, JCP 57, 3716 (1972).
- (33) Appell, Durup, Fehsenfeld, Fournier, JP B 6, 197 (1973).
- (34) Billingsley, CPL 23, 160 (1973).
- (35) Davis, Martin, Banna, Shirley, JCP 59, 4235 (1973).
- (36) Field, JMS 47, 194 (1973).
- (37) Bagus, Schrenk, Davis, Shirley, PR A 9, 1090 (1974).
- (38) Billingsley, Krauss, JCP 60, 2767 (1974).
- (39) Hertz, Jochims, Schenk, Sroka, CPL 29, 572 (1974).
- (40) Thulstrup, Thulstrup, Andersen, Öhrn, JCP 60, 3975 (1974).
- (41) Alberti, Douglas, CJP 53, 1179 (1975).
- (42) Coxon, Clyne, Setser, CP 7, 255 (1975).
- (43) Hillier, Kendrick, JCS FT II 71, 1654 (1975).
- (44) Darko, Hillier, Kendrick, CPL 45, 188 (1977).

NO⁺, NO⁺⁺,

^a $D_0^0(\text{NO}) + \text{I.P.}(\text{O}) - \text{I.P.}(\text{NO})$.

^bAverage of two values obtained by electron impact mass-spectrometry (5) and double charge transfer spectroscopy (33). A similar value (30.8 eV) can be derived from Auger electron spectra (28), but the assignments are highly tentative and can also be interpreted as indicating an ionization potential of only ~ 26 eV.

^cThe $1s_N$ and $1s_O$ $1\Pi - 3\Pi$ splittings are 1.41 and 0.53 eV, respectively (29)(35). The $1s_N$ photoelectron peaks have an anomalous intensity ratio of 3.43 (37); theoretical interpretation (43)(44). Predicted $1s_N$ satellite ("shake-up") peaks (43).

^dLong vibrational progression in the photoelectron spectrum at ~ 23 eV (21)(25); neither the vibrational numbering nor the assignment to $B^1\Sigma^+$ are certain. (26) suggests a mixed 1Π state resulting from configuration interaction between states arising from $\dots 4\sigma^2 5\sigma^2 1\pi^4 2\pi$ (like $c^3\Pi$) and $\dots 4\sigma^2 5\sigma 1\pi^3 2\pi^2$. See also (32)(40).

^eLimit of the Narayana-Price Rydberg series. Single strong peak in the photoelectron spectrum at 21.72 eV (16)(17)(21)(25). The high-energy wing is overlapped by weak unresolved structure ($\omega \approx 400$) tentatively attributed to the corresponding 1Π state by (25); see, however, ^d. Predissociation into $N^+ + O$ (39).

^fLimit of Tanaka's β Rydberg series. Short progression in the photoelectron spectrum (9)(16)(21)(25); see ^h.

^g $w_{e_y} = -0.2683$.

^hFranck-Condon factors for ionizing transitions from $X^2\Pi$ (7)(8)(11)(15)(36)(42).

ⁱPerturbations by $b^3\Sigma^-$ (4)(36)(41).

^jRadiative lifetime $\tau(v=0) = 56$ ns (10)(13); $f_{00} = 0.00025$. Variation of transition moment with r (24)(30)(31).

^kFranck-Condon factors (15)(23)(42).

^lLong upper state progression in the photoelectron spectrum (21)(25); see ^h.

^mInterpolated using data for CO and N₂ (36).

ⁿAdjusted to give agreement with $B_5 = 1.2512$ as obtained from a perturbation analysis (36).

^oFragments in emission from perturbed $A^1\Pi \sim b^3\Sigma^-$ levels.

^pLimit of Tanaka's β Rydberg series. Very short progression in the photoelectron spectrum (9)(16)(21)(25); see ^h.

^qQuadrupole moment of NO⁺ = $+0.79 \times 10^{-26}$ esu cm² (19); see also (22)(38).

^rObserved in the IR spectrum of hot air resulting from a high altitude nuclear detonation; the 1-0 and 2-0 bands have been identified. Theoretical intensities (34).

(1) Tanaka, Sci. Pap. IPCR (Tokyo) 39, 456 (1942).

(2) Baer, Miescher, HPA 26, 91 (1953).

(3) Tanaka, JCP 21, 562 (1953).

(4) Miescher, CJP 33, 355 (1955); HPA 29, 135 (1956).

(5) Dorman, Morrison, JCP 35, 575 (1961).

(6) Huber, HPA 34, 929 (1961).

(7) Wacks, JCP 41, 930 (1964).

(8) Halmann, Laulicht, JCP 43, 1503 (1965).

(9) Turner, May, JCP 45, 471 (1966).

(10) Hesser, Dressler, JCP 45, 3149 (1966).

(11) Spohr, von Puttkamer, ZN 22 a, 705 (1967).

(continued on p.481)

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{14}\text{N}^{16}\text{O}^-$		$D_0^0 = 5.056 \text{ eV}^a$ I.P. = 0.024 eV^b								MAR 1977 A	
		Evidence for additional compound states ("resonances" related to the "grandparents" $b^3\Pi$, $A^1\Pi$, and $c^3\Pi$ of NO^+) in the 12-18 eV region of the electron transmission (2)(7) and electroionization (9) spectra of NO.									
		The nature of the state (or states) involved in the production of $\text{N}(^2\text{D}) + \text{O}^-$ by dissociative electron attachment (7-12 eV) has been discussed by (11); see also (10).									
		Short vibrational progressions of resonances in the electron transmission current (2); predicted widths range from 1 to 25 meV (14).									
	$(^3\Sigma^-)^c$	51700	2320	13	}						
	$(^3\Sigma^+)^c$	43800	2380	12							
	$(^3\Pi)^c$	43400	2370	12							
	$(^1\Sigma^+)^c$	40400	2330	8							
b	$^1\Sigma^+$	(9300) ^d									
a	$^1\Delta$	6050	1492 ^d	(8)				1.26 ₂ ^d			
x	$^3\Sigma^-$	0	1363 ^d	8		1.42 ₇ ^e		1.25 ₈ ^e			
$(^{237})\text{Np}^{16}\text{O}$		$(\mu = 14.9838726_3)$ a I.P. = 5.7 eV^b								JUN 1975	
$^{14}\text{N}^{32}\text{S}$		$\mu = 9.7380289_4$ $D_0^0 = 4.8 \text{ eV}^a$ I.P. = 8.87 eV^b								MAY 1977	
		Theoretical potential curves for most of the observed valence states have been calculated by (28).									
F	$^2\Delta$					$[0.8367]^c$	$[1.05]$	$[1.438_4]$	$F \rightarrow X, \quad V$	$\begin{matrix} 55959.8 \\ 56181.3 \end{matrix}$ $\begin{matrix} Z \\ Z \end{matrix}$	(11)(29)*
J	$^2\Sigma^+$					$[(0.825)]^d$		$[(1.44_9)]$	$J \rightarrow X, \quad V$	$\begin{matrix} 55562 \\ 55784 \end{matrix}$	(29)
E	$^2\Pi_r$	e				$[0.821]^e$		$[1.45_2]$	$E \rightarrow X,$	$\begin{matrix} 51154^e \\ 51330^e \end{matrix}$	(11)(29)*
I	$^2\Sigma^+$	(44400)	[1008]			$[0.6940]^f$	[5]	$[1.579_3]$	$I \rightarrow X, \quad R$	$\begin{matrix} 44050.1 \\ 44271.6 \end{matrix}$ $\begin{matrix} Z \\ Z \end{matrix}$	(7)*(11)(15) (23)*(29)

$(^3\Pi)^c$

43400

2370

12

$(^1\Sigma^+)^c$

40400

2330

8

Short vibrational progressions of resonances in the electron transmission current (2); predicted widths range from 1 to 25 meV (14).

NO⁻: ^aFrom D₀⁰(NO) and the electron affinities of O and NO.

^bFrom the photodetachment spectrum (5). Good agreement with (3) and (4).

^cSymmetries assigned on the basis of theoretical calculations (6). The states consist of two Rydberg electrons temporarily bound to the NO⁺ X¹Σ⁺ core.

^dFrom the analysis (13)(15) of electron scattering data (1)(7)(8)(12). For the ground state (5) estimate $\omega_e \approx 1470 \text{ cm}^{-1}$, see ^e.

^eFranck-Condon factor analysis of the photodetachment spectrum (5). The analysis of electron scattering data (15) leads to $r_e = 1.267 \text{ \AA}$.

(1) Spence, Schulz, PR A 3, 1968 (1971).

(2) Sanche, Schulz, PRL 27, 1333 (1971); PR A 6, 69 (1972).

(3) McFarland, Dunkin, Fehsenfeld, Schmeltekopf, Ferguson, JCP 56, 2358 (1972).

(4) Parkes, Sugden, JCS FT II 68, 600 (1972).

(5) Siegel, Celotta, Hall, Levine, Bennett, PR A 6, 607 (1972).

(6) Lefebvre-Brion, CPL 19, 456 (1973).

(7) Schulz, RMP 45, 423 (1973).

(8) Burrow, CPL 26, 265 (1974).

(9) Carbonneau, Marmet, CJP 52, 1885 (1974).

(10) Thulstrup, Thulstrup, Andersen, Øhrn, JCP 60, 3975 (1974).

(11) Van Brunt, Kieffer, PR A 10, 1633 (1974).

(12) Zecca, Lazzizzera, Krauss, Kuyatt, JCP 61, 4560 (1974).

(13) Tronc, Huetz, Landau, Pichou, Reinhardt, JP B 8, 1160 (1975).

NO⁻ (continued):

(14) Pearson, Lefebvre-Brion, PR A 13, 2106 (1976).

(15) Teillet-Billy, Fiquet-Fayard, JP B 10, L111 (1977).

NpO: ^aThermodynamic properties of NpO (1).

^bCorrected electron impact appearance potential (2).

(1) Ackermann, Rauh, JCP 62, 108 (1975).

(2) Rauh, Ackermann, JCP 62, 1584 (1975).

NS: ^aEstimate based on a linear Birge-Sponer extrapolation for the ground state (19). Ab initio calculations (19) give 5.2 eV.

^bFrom the photoelectron spectrum (30).

^cIntensity perturbations and predissociations in both doublet components.

^dOnly fragments observed.

^eApproximate deperturbed constants, $A \approx +45$. This level is strongly perturbed by $v=11$ of H ²Π₁ ($B_{11} = 0.525$, $A_{11} = -110$).

^fSpin doubling constant $\gamma_0 \approx +0.1$ for $N \leq 20$. The spin splitting increases rapidly at higher N because of a perturbation by H ²Π($v=1$). I ²Σ⁺($v=1$) ($B_1 \approx 0.695$) interacts with H ²Π($v=2$) at somewhat lower N values. A strong homogeneous interaction with levels of C ²Σ⁺ explains the larger than expected $\Delta G(\frac{1}{2})$ value of I ²Σ⁺.

(References on p. 487)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^{32}\text{S}$ (continued)										
H $^2\Pi_i$	(44049) ^g 43876	767.6	5.0	[0.5972] [0.5915] h	0.0059	[1.75]	1.702	H \rightarrow X, R	43824.6 43429.6 Z	(21)* (23) (29)
C $^2\Sigma^+$	43290	[1389]	i	[0.8275]	i	[1.2]	[1.446 ₄]	C ^j \leftrightarrow X, ^k V γ system	43165.9 43387.4 Z	(1)(2)* (3) (6)* (15) (24)* (29)*
G $^2\Sigma^-$	43346	[879.8]	Z	[0.6905] ^l	m	[2.5]	[1.583 ₄]	G \rightarrow X, R	42956.8 43178.3 Z	(23)*
A $^2\Delta_r$	(40046) 40005	[934.4] [943.9]	Z Z	n 8.4 H [0.6850]	n n		[1.589 ₇]	A \leftrightarrow X, ^k R β system	39688.1 39875.7 Z	(1)(4)(6)* (15)(23)*
B* $^2\Sigma^+$	(36255)	(1060)	(15)	(0.78) ^o			(1.49)	B* \rightarrow X, (35952) ^o (36174) ^o		(26)(27)
B $^2\Pi_r$	30384.1 30294.9	798.78 797.31 Z	Z	3.59 3.72	0.6013 ^p 0.5962 ^p	0.0046 0.0048	1.3 1.3	B \rightarrow X, R	29953.6 30085.1 Z	(8)(9)(12)* (13)(15)* (18)(23)*
X $^2\Pi_r$	221.5 ^q 0	1218.7	Z	7.28	[0.775156] [0.769602] ^r	0.0063 ₅	1.2	1.4940 ₂	Microwave sp. ^s EPR sp. ($^2\Pi_{3/2}$)	(16) (10)(14)(17)
$^{14}\text{N}^{32}\text{S}^+$										
$D_0^0 = 6.3 \text{ eV}^t$										MAY 1977
Bands previously (5) attributed to NS ⁺ have been reclassified by (23) as G \rightarrow X system of NS.										
X $^1\Sigma^+$	0	1415 ^u	15				1.440 ^v			
NS^-										
<u>Ab initio</u> calculations (22).										MAY 1977

NS (cont'd), NS⁺, NS⁻:

$$^gA_0 = -172.3.$$

^hPerturbations by levels of E, I, C; see e, f, i.

$$^i\Delta G(3/2) = 1414 \text{ (29)}, \Delta G(5/2) \approx 1372, \Delta G(7/2) \approx 1378 \text{ (11)}.$$

$$B_1 \approx 0.7975, B_2 = 0.8150 \text{ (29)}; (24) \text{ give } B_0 = 0.82876 \text{ and}$$

$D_0 = 1.40_4 \times 10^{-6}$ as well as $\gamma_0 = +0.0055$. C $^2\Sigma^+$ interacts strongly with I $^2\Sigma^+$; in addition, $v=1$ is extensively perturbed by H $^2\Pi(v=2)$ and G $^2\Sigma^-(v=2)$.

^jEstimated lifetime $\tau(v=0) \approx 6.5 \text{ ns}$ [Hanle effect measurements (25)].

NS, NS⁺, NS⁻ (continued):

^kObserved in absorption by (20) following the flash photolysis of OCS in the presence of excess N₂O.

^lSpin doubling constant $\gamma_0 = +0.034$.

^mB₁ = 0.6780.

ⁿThe A state is strongly perturbed, particularly the $^2\Delta_{5/2}$ component [see (23)]; the $\Delta G(\frac{1}{2})$ values are from (4), $\omega_e x_e$ from (6), and B₀ from (23). Additional constants may be found in these references but, because of the perturbations, have limited meaning. (23) suggest that the perturbing state is $^2\phi_{5/2}$.

^oOnly the 1-0 band has been observed and analyzed (B₁ = 0.7716, $\nu_0 = 37203.9$ and 36982.5). The v=0 level of $^{14}\text{N}^{32}\text{S}$ interacts with B $^2\Pi_1(v=8)$ (27); weak emission from this level was observed for $^{15}\text{N}^{32}\text{S}$ (27).

^pSeveral perturbations. Except for v=8 (see ^o), these interactions have not yet been analyzed.

^qA₀ = + 222.9₄, A₁ = + 223.0₉, recalculated by (16) from the data of (2).

^r Λ -type doubling, $\Delta\nu_{fe}(v=0) = +0.01325_3(J+\frac{1}{2})$ (16).

^s $\mu_{el}(^2\Pi_1, v=0) = 1.81$ D from Stark effect measurements in the rotation spectrum (16); (14), using the EPR method, obtained 1.3₅ D for $^2\Pi_{3/2}$. This value was recently revised to 1.86 D (31). See also (19). Hyperfine coupling constants (14)(16)(17).

^tD₀(NS) + I.P.(S) - I.P.(NS).

^uVibrational constants from the photoelectron spectrum (30).

^vEstimated value from a Franck-Condon factor analysis of the photoelectron peaks (30).

(1) Fowler, Bakker, PRS A 136, 28 (1932).

(2) Zeeman, CJP 29, 174 (1951).

(3) Barrow, Downie, Laird, PPS A 65, 70 (1952).

(4) Barrow, Drummond, Zeeman, PPS A 67, 365 (1954).

(5) Dressler, HPA 28, 563 (1955).

(6) Narasimham, Srikameswaran, PIAS A 56, 316 (1962).

(7) Narasimham, Srikameswaran, PIAS A 56, 325 (1962).

(8) Narasimham, Srikameswaran, PIAS A 59, 227 (1964); Nature

(9) Smith, Meyer, JMS 14, 160 (1964). | 197, 370 (1963).

(10) Carrington, Levy, JCP 44, 1298 (1966).

(11) Joshi, ZP 191, 126 (1966).

(12) Peyron, Lam Thanh My, JCPPB 64, 129 (1967).

(13) Goudmand, Dessaux, JCPPB 64, 135 (1967).

(14) Carrington, Howard, Levy, Robertson, MP 15, 187 (1968).

(15) Narasimham, Subramanian, JMS 29, 294 (1969).

(16) Amano, Saito, Hirota, Morino, JMS 32, 97 (1969).

(17) Uehara, Morino, MP 17, 239 (1969).

(18) Vidal, Dessaux, Marteel, Goudmand, CR C 268, 2140 (1969).

(19) O'Hare, JCP 52, 2992 (1970).

(20) Donovan, Breckenridge, CPL 11, 520 (1971).

(21) Narasimham, Balasubramanian, JMS 40, 511 (1971).

(22) O'Hare, JCP 54, 4124 (1971).

(23) Jenouvrier, Pascat, CJP 51, 2143 (1973).

(24) Balasubramanian, Narasimham, JMS 53, 128 (1974).

(25) Sivers, Chiu, JCP 61, 1475 (1974); JMS 61, 316 (1976).

(26) Narasimham, Raghuveer, Balasubramanian, JMS 54, 160 (1975).

(27) Jenouvrier, Daumont, JMS 61, 313 (1976).

(28) Bialski, Grein, JMS 61, 321 (1976).

(29) Vervloet, Jenouvrier, CJP 54, 1909 (1976).

(30) Dyke, Morris, Trickle, JCS FT II 73, 147 (1977).

(31) Byfleet, Carrington, Russell, MP 20, 271 (1971).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{14}\text{N}^{80}\text{Se}$										
		$\mu = 11.9152663_g$		$D_0^0 = (4.0) \text{ eV}$						MAY 1977
C $^2\Delta_{5/2}$	(34650)	$\Delta G(3/2) = 738.32$		$B_2 = 0.4410$ $B_1 = 0.4568$		$2.5 (D_2)$ $0.01 (D_1)$ $r_1 = 1.760$		$C \rightarrow X_2, ^a R$ $v(1-0) = 34431.48 \text{ Z}$		(8)(12)* (13)*
B $^2\Sigma(-)$	(34400)	b		$[0.4503]^c$		$[2.8]$ $[1.772_5]$		$B \rightarrow X_2, ^d R$ 33431.21 Z $B \rightarrow X_1, ^d R$ 34322.03 Z		(12)(13)*
b ($^4\Sigma_{1/2}^-$)	(24840)	$[766] \text{ H}$		$[0.4407]^e$		$[1.791_7]$		$b \rightarrow X_1, ^f R$ 24744.3 H		(16)
A ₂ $^2\Pi_{3/2}$	(24800)	$[612.5] \text{ Z}$ g		$[0.4173]$ g		$[0.67]$ $[1.841]$		$A_2 \rightarrow X_2, ^h R$ 23765.4 Z		(9)* (16)*
A ₁ $^2\Pi_{1/2}$	(24350)	$[658.9] \text{ Z}$ i		$[0.4117]$ i		$[0.60]$ $[1.854]$		$A_1 \rightarrow X_1, ^h R$ 24204.0 Z		(9)* (16)*
a ($^4\Pi_i$)	(19700) ^j	$(710.7)^j$ $(10.3)^j$		$(0.361)^j$ $(0.002)^j$		(1.98_0)				
X ₂ $^2\Pi_{3/2}$	891.8 ^k	954.96 Z 5.64 ₈		0.5189 0.0040		0.65				
X ₁ $^2\Pi_{1/2}$	0	956.81 Z 5.64 ₃		0.5182 ^l 0.0040		0.65		1.6518		

NSe: ^a(12) originally assigned the $v'=1$ progression to a $^2\Pi_{1/2} \rightarrow X_1^2\Pi_{1/2}$ transition.

^bA weak band at 2845.37 Å was assigned by (12) to the $B \rightarrow X_1$ 1-0 transition, giving $\Delta G'(\frac{1}{2}) = 804.6$.

^cSpin splitting constant $\gamma_0 = -0.035$.

^d(8) assigned the $v'=0$ progression to a $^2\Pi_{1/2} \rightarrow X_1^2\Pi_{1/2}$ transition. These authors list a number of unclassified bands in the same wavelength region.

^eCalculated from the corresponding value for $^{15}\text{N}^{80}\text{Se}$. The b state levels interact with $A_1^2\Pi_{1/2}$, see ⁱ.

^fTwo very weak v'' progressions.

^gStrongly perturbed state; $\Delta G(3/2) = 803.8$, $\Delta G(5/2) = 654.4$, $\Delta G(7/2) = 637.7$; $B_1 = 0.4252$, $B_2 = 0.4164$, $B_3 = 0.4112$, $B_4 = 0.4069$. According to (16) the perturbing state may well be $^4\Sigma_{3/2}^-$.

^hEarlier assignments of bands belonging to these two subsystems postulated the existence of two close lying and interacting $^2\Pi$ states called $A^2\Pi_{1/2}$, $A'^2\Pi_{1/2}$, and $A, A'^2\Pi_{3/2}$; see (14), also (1)(2)(3)(4)(5)(6)(7)(10)(11). (16) use A and A' in place of A_1 and A_2 , respectively.

ⁱStrongly perturbed state; $\Delta G(3/2) = 615.8$, $\Delta G(5/2) = 695.7$; $B_1 = 0.4096$, $B_2 = 0.4205$, $B_3 = 0.4093$, $B_5 = 0.3980$, $B_7 = 0.3920$, $B_8 = 0.3901$. Λ -type doubling $\Delta v(v=0) = 0.032(J+\frac{1}{2})$, the sign being opposite to that in $X_1^2\Pi_{1/2}$. For higher vibrational levels the Λ -type doubling is irregular owing to the strong interaction with $b^4\Sigma_{1/2}^-$.

^j $A \approx -25$; all constants have been derived from the analysis of perturbations in the A_1 , A_2 states of $^{15}\text{N}^{80}\text{Se}$ and $^{14}\text{N}^{80}\text{Se}$; see (16).

^k $A_{\text{eff}} = 890.84$ as given in (13) corresponds to the difference between the two hypothetical $J=0$ levels.

^l Λ -type doubling $\Delta v = 0.043(J+\frac{1}{2})$. The interaction (due to s-uncoupling) between the nearly degenerate levels $v+1$ and v of $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$, respectively, leads for $v = 4, 5$ to an anomalous Λ -type doubling in both components (15).

- (1) Pannetier, Goudmand, Dessaux, Arditi, CR 260, 2155 (1965).
- (2) Goudmand, Dessaux, JCPPB 64, 135 (1967).
- (3) Dessaux, Goudmand, CR C 267, 1198 (1968).
- (4) Pascat, Daumont, Jenouvrier, Guénébaut, CR B 269, 1309 (1969).
- (5) Pascat, Daumont, Jenouvrier, Guénébaut, CR C 270, 20 (1970).
- (6) Daumont, Jenouvrier, Pascat, Guénébaut, CR B 271, 120 (1970).
- (7) Daumont, Jenouvrier, Pascat, CR C 271, 712 (1970).
- (8) Jenouvrier, Daumont, Pascat, CR C 271, 1358 (1970).
- (9) Subbaram, Rao, JMS 36, 163 (1970).
- (10) Daumont, Jenouvrier, Pascat, Guénébaut, CR C 272, 1545 (1971).
- (11) Jenouvrier, Daumont, Pascat, Guénébaut, CR C 272, 1627 (1971).
- (12) Yee, Jones, JMS 37, 304 (1971).
- (13) Harding, Jones, Yee, Jenouvrier, Daumont, Pascat, Guénébaut, CJP 42, 2033 (1971).
- (14) Daumont, Jenouvrier, Pascat, Guénébaut, JCPPB 69, 218 (1972).
- (15) Jenouvrier, Pascat, Lefebvre-Brion, JMS 45, 46 (1973).
- (16) Daumont, Jenouvrier, Pascat, CJP 54, 1292 (1976).

State	T_e	w_e	w_{ex_e}	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{16}O_2$		$\mu = 7.9974575_1$		$D_0^0 = 5.115_6$ eV ^a						MAR 1977 A
		A detailed review of the entire spectrum of molecular oxygen has been published by (141).								
						I.P.($1\pi_g$) = 12.071 eV ^b ($1\pi_u$) = 16.092 eV ^c ($3\sigma_g$) = 18.159 eV ^c ($2\sigma_u$) = 24.549 eV ^c ($2\sigma_g$) = 39.6 eV ^d ($1s_0$) = 543.1 eV ^d				
		Potential energy diagrams (63)(128)(141)(190); predicted electronic states and potential functions (167)(176)(182).								
Z ($^3\Pi_u$)						Several Rydberg states converging to the oxygen K limits at 543.1($^4\Sigma^-$) and 544.2($^2\Sigma^-$) eV, in X-ray absorption and electron energy loss spectra. Strong X-ray absorption peak (excitation $1s_0 \rightarrow 1\pi_g$).		Z ← X, 532 eV ^e		(133)(166) (175)
		Absorption cross sections and cross sections for the production of atomic fluorescence by photodissociation in the region 175-850 Å (570000-115000 cm $^{-1}$) (156)(158)(161)(164). Earlier results in (18)(23)(58).								
						Rydberg states with the outer electrons in $3s\sigma$, $3p\sigma$, $3d\sigma$ orbitals and the O_2^+ core in the highest ... $1\pi_u^3 1\pi_g^2 2\Pi_u$ state have been tentatively identified in the electroionization spectrum of O_2 at 20.73, 21.75, 22.28 eV, respectively.				(160)
						Codling and Madden's Rydberg series converging to c $^4\Sigma_u^-(v=0)$ of O_2^+ :				
						$v = 198125 - \begin{cases} R/(n-0.16)^2 & n = 3(Y \text{ state}), 4 \dots 11. f g \\ R/(n-0.95)^2 & n = 3(W \text{ state}), 4 \dots 8. f g h \end{cases}$				(65)*
Y ^f (184440)						[1510]		Y ← X, 184410		(65)*
W ($^3\Sigma_u^-$) ^f (168290)						[1510]		W ← X, 168260		(65)*
						Yoshino and Tanaka's weak Rydberg series converging to B $^2\Sigma_g^-(v=0)$ of O_2^+ :				
						$v = 163700 - R/(n-0.54)^2$				(98)
V ^f (160270)						(1100)		V ← X, 160031		(98)
						Tanaka and Takamine's strong Rydberg s. of R shaded dif. b. converging to B $^2\Sigma_g^-(v=0)$ of O_2^+ :				
						$v = 163702 - R/(n-0.70)^2$				(9)(86)*(98)*
						$n = 3(U \text{ state}), 4 \dots 23. f i$				

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
¹⁶ O ₂ (continued)										
Fragments of Rydberg series (155000 - 160000 cm^{-1}) converging to D ² Δ_g of O ₂ ⁺ .										(93)
Namioka, Ogawa and Tanaka's Rydberg s. of weak R shaded b. converging to b ⁴ $\Sigma_g^-(v=0)$ of O ₂ ⁺ , $v = 146560^j - R/(n - 0.53)^2 \quad n = 4$ (R state), 5...16. ^f Similar series with $v'=1.2$.										(44)(98)*
Tanaka and Takamine's Rydberg s. of strong R shaded b. converging to b ⁴ $\Sigma_g^-(v=0)$ of O ₂ ⁺ , $v = 146556^j - R/(n - 0.68)^2 \quad n = 4$ (Q state), 5...30. ^{f,k} Similar series with $v'=1...4$.										(9)(44)(98)*
U	f	142548	1148	H	23			U ← X,	R 142329	H (9)(86)
R	f	(137643)	(1152)	H				R ← X,	R 137432	H (98)
Q	f	136759	1207	H	18			Q ← X,	R 136571	H (6)(44)(98)

O₂: ^a $= 41260 \pm 15 \text{ cm}^{-1}$, from the convergence limit of the B ← X bands (21).

^bFrom the high-resolution photoelectron spectrum of (178), see also (60)(72)(97). Photoionization studies [(73)(75), additional references in (178)] give appearance potentials of $\sim 12.067 \text{ eV}$.

^cCalculated from the energy levels of O₂⁺.

^dFrom the X-ray photoelectron spectrum (112).

^e(166) obtain 530.8 eV from the electron energy loss spectrum.

^fPossible upper state symmetries have been discussed on theoretical (81) and empirical (93) grounds. Several of these Rydberg levels have also been observed in the high-resolution electron energy loss spectrum (99).

^gStrongly preionized.

^hA weak satellite series approximately 50 cm^{-1} longward of the main bands has been observed by (65).

ⁱPreionization observed by photoionization mass-spectrometry (170).

^jThe limits refer to band origins; the approximate head-origin separation has been subtracted from the observed heads.

^kBoth preionization (to O₂⁺ + e⁻) and predissociation (to O⁺ + O⁻, for $n \geq 5$) have been established by photoionization mass-spectrometry (170).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
¹⁶ O ₂ (continued)										
i (¹ Δ_{2u})	(86846)	[2062]		[1.688]	0.042	[10.5]	[1.117]	i } $\leftarrow a, v$	79208.0 ^m Z	(84)(146)
i' (³ Δ_{2u})	(86843)	[1699]		[1.791]		[140]	[1.085]	i' }	79022.6 ^m Z	(152)
h (¹ Π_u)	(86750)	(2200)		[1.451] ⁿ			[1.205] ⁿ	h $\leftarrow a, v$	81362.5 ⁿ Z	(84)(146)
g (¹ Π_u)	(86604)	[2048]		[1.615] ^o		[6.0] ^o	[1.142]	g $\leftarrow X, v$	86841.4 Z	(151)

- O₂: ^aThe 0-0, 1-0, 2-0 bands are overlapped. Vibrational numbering confirmed by ¹⁸O₂ isotope shifts.
- ^bRotational analyses for v=3,5,7; v=4,6,8,9 are diffuse.
- ^cProbably progression II of (9), extended and reassigned by Katayama, Huffman, Tanaka [unpubl., see Figure 1 of (170)].
- ^dPreionization observed by photoionization mass-spectrometry (170). Several autoionizing levels have been studied by photoelectron spectroscopy (123)(155)(157). See also (47).
- ^eThese progressions have been reassigned and extended by Katayama, Huffman, Tanaka (see ^c) and include most of the bands of progressions I, N, I', P of (6). They occur in the region of the second member (4s σ_g) of the Rydberg series beginning with H [(93), see ^g]. Other Rydberg series going to a⁴ Π_u or A² Π_u may also be present; higher members possibly account for many unassigned bands in the region 810-740 \AA (123000-135000 cm^{-1}).
- ^fThat the diffuse nature of the bands is at least partly due to predissociation has been shown by the observation of O I lines in fluorescence; (161) gives cross sections for this reaction from 850 to 650 \AA (117000-154000 cm^{-1}).
- ^gLong but strongly perturbed v' progression composed of bands previously (6) assigned to four shorter progressions H, H',

- M, M'; first member (3s σ_g) of a Rydberg series converging to a⁴ Π_u of O₂⁺ (93)(195). The intensity distribution [(53) (82), see also (170)] closely resembles that of the a⁴ Π_u progression in the photoelectron spectrum (195).
- ^hVibrational numbering uncertain.
- ⁱ(111) assumed this to be a ³ Σ_u^+ state; reassigned by (151). $J_{B_1} = 1.698$, $D_1 = 42 \times 10^{-6}$.
- ^kPartial rotational analyses of a weak and diffuse 0-0 band and of stronger 1-0 and 2-0 bands (151).
- ^lThe ¹⁸O₂ isotope effect shows that this is a 0-0 band (173).
- ^mThe two components are assumed to correspond to the ground state splitting (A=200) of O₂⁺ (146)(152).
- ⁿPerturbed rotational structure. According to (146) these constants refer to the 1-0 band, the unresolved 0-0 band being at 79180 cm^{-1} .
- ^oConstants for Π^+ ; $B_0(\Pi^-) = 1.611$, $D_0(\Pi^-) = 14 \times 10^{-6}$. Constants for the diffuse v=1 level were also determined.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{16}\text{O}_2$ (continued)										
F'	[87510]	Group of six line-like features similar to F \leftarrow X.						F' \leftarrow X,	86720	(17)(173)*
F $^3\Pi_u$	(85868)	[2008]	H	v=1 diffuse	[1.434]	[11]	[1.212]	F \leftarrow X,	86085.0	a Z (136)(151)
	(85780)	[2000]	H		[1.398]	[6.0]	[1.228]		85992.6	a Z (173)*
	(85689)	[2001]	H		[1.352]	[5.3]	[1.249]		85902.3	Z (6)*(17)
E $^3\Sigma_u^-$	(79883)	[2547]	b		b			E \leftarrow X,	R 80369 ^b	(150)(173)*
f $^1\Sigma_u^+$ ^c	76091	1927	19.0		1.703 ^d	0.020	e	f \leftarrow b,	V 63141.5	Z (84)
								f \leftarrow X,	V 76262.4 ^f	(84)(111)*
										(173)*
D ($^3\Sigma_u^+$) ^g	(75260)	1957	19.7		1.73 ^h	0.025	i	D \leftarrow X,	V (75450)	(84)(111)*
e ($^1\Delta_{2u}$)	(75254)	[1830]	H		[1.682]	(diffuse lines)		e } \leftarrow a,	V 67499.6 ^k	Z (84)(118)
e' ($^3\Delta_{2u}$)	(74915)	[2052]	H	j				e' }	V 67272	k H (146)(152)
d ($^1\Pi_g$)	(69180)	[1860]		l				(d \leftarrow X)	69320 ^m	(192)
C ($^3\Pi_g$)	(65530)	[1840]		n				(C \leftarrow X)	65670 ^m	(150)(171)
B $^3\Sigma_u^-$	49793.28	709.31 ^o	Z	10.65 ^o	0.81902 ^{opq}	0.01206 ^o	4.55 ^r	1.60426	B \leftrightarrow X, st R 49358.15	Z (5)*(7)*(21)*
									Schumann-Runge b.	(78)* (96)*
										(115)(168)

O_2 : ^aThe $^{18}\text{O}_2$ isotope shift shows that this is a 0-0 band. F $^3\Pi_u$ is a mixed state resulting from the avoided crossing of the unstable $^3\Pi_u$ state (arising from $^3p+^3p$) with the lowest $^3\Pi_u$ Rydberg state ($3p\sigma_u$); see (167)(194). Oscillator strengths (171).

^bThe three strongest bands in this region at 80369, 82916, 85345 cm^{-1} [called "longest band", "second band", "third band" by (17)] have long resisted attempts at identification. Recent ab initio calculations (186)(194) have shown that very probably they correspond to the second $^3\Sigma_u^-$ state

formed by the avoided crossing of B $^3\Sigma_u^-$ with the lowest $^3\Sigma_u^-$ Rydberg state ($3p\pi_u$). The predicted ω_e is of the order of 3000 cm^{-1} . All three bands are diffuse [^1D atoms have been detected in the predissociation of E $^3\Sigma_u^-$ (193)] and show double peaks (two close double peaks for the "second band"). In $^{18}\text{O}_2$ the rotational structure of the "longest band" is resolved [$B'=1.307_2$, $D'=1.8 \times 10^{-6}$, $\lambda'=-3.3_7$, $\gamma' = +0.045$ (179)] and confirms that the upper state is indeed $^3\Sigma_u^-$ (173). On the basis of the observed isotope shift (173) prefer the assignment of the "longest band" as 1-0 b. [see

O₂ (continued):

also (194)]. *f* values of 0.0102, 0.0080, 0.0015 for the three bands have been determined from electron energy loss measurements (171).

^c α state of (84), progression II of (17).

^d $v=2$ diffuse. Rotational constants for $^{18}\text{O}_2$ in (179).

^e $D_2 = 25.8 \times 10^{-6}$, $D_3 = 7 \times 10^{-6}$, $D_4 = 10 \times 10^{-6}$.

^fThe 0-0 band is not observed since it is in the continuum which covers the 1300 Å region.

^g β state of (84) who assumed it to be $^1\Sigma_u^+$; reassigned by (111). Progression I of (17).

^hLevels other than $v=2$ and 3 are too diffuse for analysis, both in $^{16}\text{O}_2$ and $^{18}\text{O}_2$; for the latter see (179).

ⁱ $D_2 = 14.8 \times 10^{-6}$, $D_3 = 21.0 \times 10^{-6}$.

^j $\Delta G(3/2) = 1698$, $\Delta G(5/2) = 1838$.

^kSee ^m on p. 493.

^l $\Delta G(3/2) = 1770$, $\Delta G(5/2) \approx 1800$.

^mFrom electron energy loss spectra. C and d are considered to be the lowest Rydberg states ($3s6g_g$) of O₂. Apparent oscillator strengths, summed over the first four bands of the C-X progression, yield an *f* value of 0.00074 (171).

ⁿ $\Delta G(3/2) = 1960$, $\Delta G(5/2) = 1780$ [average of values given by (150) and (171)].

^o $\omega_e y_e = -0.139$, $r_e = -0.000556$, from a low order fit to $v \leq 4$; the representation of levels having $v \leq 13$ requires seven Y_{10} and seven Y_{11} coefficients (141)(190). Band origins ($v''=0$), B_v , D_v values for $v'=0 \dots 21$ (115)(168)(190); T_0 values of (115) (absorption) and (168) (emission) agree to better than 0.1 cm^{-1} [note, however, two typographical errors for G_0 and G_3 in Table 5 of (168)]. Convergence limit of the vibrational levels at 57127.5 cm^{-1} (21). RKR potential (141)

^pThe spin splitting constants at low v are $\lambda = 1.5$, $|$ (37)(64). $-f \approx 0.04 \text{ cm}^{-1}$. They increase rapidly above $v \approx 12$ (21)(135).

^qPredissociation above $v=2$ established by line width measurements in absorption (27)(31)(92)(115)(119)(139); maximum at $v=4$, subsidiary peaks at $v=7, 11$. Ab initio calculations (134)(174)(185) show that the repulsive $^5\Pi_u$ state from normal atoms is the main contributor to the predissociation with smaller contributions from $^1\Pi_u$, $^3\Pi_u$ [earlier investigators assumed this to be the only contributor (101)(110)(114)(125)] and $^3\Sigma_u^+$. Evidence for inverse predissociation has been found by (95); see also (122)(131).

^r $\beta = +0.22 \times 10^{-6}$ for low v ; D_v increases rapidly above $v \approx 4$.

^sThe B state levels have been observed in absorption from $v'=0$ to the convergence limit (see ^o) (21)(115). Absorption by vibrationally excited O₂ ($v'' \leq 5$) (74)(96); data for $^{17}\text{O}^{16}\text{O}$, $^{18}\text{O}^{16}\text{O}$, $^{18}\text{O}_2$ (52)(61); absorption in inert gas matrices (58a)(63a)(115a) and (197). The formation of O(¹D) atoms by photoabsorption in the adjoining continuum has been verified by (193). Emission bands with low v' and high v'' are observed in various electrical discharges (13)(39)(168).

^tFor intensity measurements in the discrete portion of the B-X system see (30a)(69)(90)(92)(113)(117)(171), and in the continuum (68)(69)(71)(171); at the absorption maximum near 1445 Å (69200 cm^{-1}) the absorption coefficient is 382 cm^{-1} ($\sigma = 1.42 \times 10^{-17} \text{ cm}^2$) (71). Absorption *f* values vary from 3.4×10^{-10} for the 0-0 band to 3.4×10^{-5} for the 14-0, 15-0 bands to 1.3×10^{-5} for the 20-0 band, yielding an oscillator strength sum of $\sim 32 \times 10^{-5}$ for the Schumann-Runge bands. The overall electronic absorption oscillator strength is 0.162 which represents an upper limit if, as suggested by (171) and recently confirmed by (196), the continuum contains contributions from other dissociative states; see (continued on p. 497)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions Design. ν_{00}	References
$^{16}\text{O}_2$ (continued)									
A $^3\Sigma_u^+$	35397.8	799.07	Z 12.16 ^a	0.9106	0.0141 ₆ ^a	4.7 ^b	1.5215	(A \rightarrow b) ^c (21886) (A \rightarrow a) ^c (27125) A \leftrightarrow X, ^{de} R 35007.1 ₅ Z Herzberg I b.	(16)* (22)* (89)*
A' $^3\Delta_u$	(34690) ^f	(850) ^g	(20) ^g	(0.96) ^h	(0.026 ₂) ^h		(1.48)	(A' \rightarrow a) ^c (26440) A' \leftrightarrow X, ^{ij} R (34320) ^g Herzberg III b.	(19)*
c $^1\Sigma_u^-$	33057.3	794.2 ₉	Z 12.73 ₆ ^k	0.915 ₅	0.0139 ₁ ^k	[7.4]	1.517 ₄	c \rightarrow a, ^l (24782) c \leftrightarrow X, ^m R 32664.1 Z Herzberg II b.	(188) (19)* (87)

O_2 : ^a $\omega_e y_e = -0.550$, ^y $\gamma_e = -0.00097$. The constants of (16) have been adjusted (80)(141) to the revised vibrational numbering (v' raised by one unit) of (22). The spin splitting constants for low v are $\lambda = -4.9_5$ and $\gamma \approx 0$; they decrease appreciably above $v \approx 7$. RKR potential (37) (89)(140)(141).

^b D_v increases rapidly above $v \approx 4$.

^cThe tentative identification of the A \rightarrow b transition in an oxygen afterglow by (22) was not confirmed by (26). Other unidentified features in the nightglow and in the oxygen afterglow have been variously attributed to the A \rightarrow a and A' \rightarrow a transitions by (189) and (28), respectively. A high resolution trace of one of these bands at 4007 \AA can be seen in Figure 1 of (87).

^dFirst observed in absorption at atmospheric pressure and

a path of > 25 m (4a)(16). The bands occur in emission in the nightglow (24)(28) and in various afterglows (22)(26) (42)(88). According to (34)(58a) bands correlated with this system have also been observed in matrix isolation studies; these bands have recently been reassigned, see ^j.

^eFor detailed intensity measurements in the discrete region and in the adjoining continuum see (43)(69)(104)(127)(129). The electronic absorption oscillator strength is $\sim 10^{-7}$; cross sections in the continuum vary from $\sim 0.5 \times 10^{-24} \text{ cm}^2$ at 2400 \AA to $\sim 30 \times 10^{-24} \text{ cm}^2$ at 1920 \AA where transitions to other dissociative states begin to make significant contributions to the observed intensity (129). Franck-Condon factors and Franck-Condon densities (80)(89)(140)(141).

^fThe separation of the F_3 and F_2 components in $v=6$, extrapolated to $J=0$, is 145.9 cm^{-1} .

O₂ (continued):

^εThe vibrational constants and ν_{00} have been estimated from measurements of the diffuse high-pressure bands (see ⁱ). The only accurately known vibrational interval is $\Delta G(5\frac{1}{2}) = 611.2$ for the F₃ component (19). The vibrational numbering is uncertain.

^hExtrapolated from B₅ and B₆ assuming a linear B_v curve; the ν numbering has been estimated (see ^g).

ⁱOnly two weak bands have been analyzed at low pressure and 800 m path length (19). At high pressure and in liquid O₂ a fairly strong progression of diffuse triplets has been studied by many investigators. This progression appears to be the analogue in (O₂)₂ of the A'←X bands (their intensity increases with the square of the pressure) (1)(4)(8)(19). For lack of other information the A'←X 0-0 band is assumed to be at the position of the first diffuse high-pressure band.

^jVisible emission bands of oxygen in low temperature matrices (34) have recently been reinterpreted (188) as belonging to the A'←X system.

^k $\omega_e \nu_e = -0.244_4$, $\omega_e z_e = +0.0005_5$; $y_e = -0.00074_0$. The constants refer to the revised vibrational numbering suggested by (87); see ^m.

^lThis system was only observed in Xe matrices ($\nu_{00} = 24552$) by excitation with VUV light.

^mIn absorption the 6-0,...,11-0 bands [new ν' numbering of (87), 1-0,...,6-0 in the old numbering of (19)] have been observed with path lengths of 800 m atm (19); in emission several bands with low ν' are seen in the afterglow of an oxygen-argon mixture (70)(87). The $\nu'=0$ progression is the strongest feature of the Venus night airglow (191).

O₂ (continued from p. 495):

also (187). A rather different total f value of 0.040 is derived from shock-tube absorption and emission studies (33)(51)(103); the discrepancy is probably due to the r -dependence of the electronic transition moment (56)(77)(121)

(187). Franck-Condon factors based on RKR and similar potentials (50)(77)(106)(141)(190); (77) give data for ¹⁸O₂. The spectral emissivity in the Schumann-Runge bands has been discussed by (85)(103). Franck-Condon densities (55).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
¹⁶ O ₂ (continued)										
b $1\Sigma_g^+$	13195.1	1432.77 ^a	Z 14.00 ^a	1.40037 ^a	0.01820 ^a	5.351 ^b	1.22688	b→a, ^c 5238.5	(40)	
								b↔X, ^{de} R 13120.91 ^f Z	(12)*	
								Atmospheric oxygen b.		
a $1\Delta_g$	7918.1	[1483.5 ₀]	Z (12. ₉)	1.4264	0.0171	[4.86]	1.2156 ₃	a↔X, ^{he} R 7882.39 Z	(10)*	
								IR atmosph. oxygen b.		
X $3\Sigma_g^-$	0	1580.19 ₃	Z 11.98 ₁ ⁱ	[1.4376766] ^j B _e = 1.44563	0.0159 ₃ ^{kl}	[4.839] ^{jl}	1.20752	Rot.-vibr. sp. (collision induced)	(12a)(75a) (142)	
								Rotation sp. ^{mn}	(94)(105)	
								Spin reorientation (fine structure) sp. ^{mo}	(20)(41)(76) (120)(159)	
								Raman sp. ^p	(38)* (124)* (162)(183)*	
								EPR sp.	(25)(138)(154)	

O₂: ^aThese constants have been re-evaluated [(148), see also (168)] from the measurements of the b-X system (12) using improved lower state constants; $\gamma_e = -0.00004_2$. RKR potential curve (148). Constants for $^{16}\text{O}^{18}\text{O}$, $^{16}\text{O}^{17}\text{O}$ in (12).

^b $+0.0318(v+\frac{1}{2})+0.0012(v+\frac{1}{2})^2$. The D_v values have been calculated (148) using vibrational wavefunctions computed from the experimental potential curve; see (147).

^cQ branch of the 0-0 band observed in a discharge through O₂ and He. Absolute transition probability $\sim 2.5 \times 10^{-3} \text{s}^{-1}$.

^dIn absorption observed in the solar spectrum; in the laboratory with more than 1 m path. In emission in the aurora and nightglow (14) as well as in various discharges (11) (15)(39)(40). Band intensities [in $\text{cm}^{-1}\text{km}^{-1}\text{atm}^{-1}(\text{STP})$] for

the 0-0, 1-0, 2-0 bands are 532, 40.8, 1.52, respectively (102); slightly smaller values in (137). The transition probability for the 0-0 band is 0.075s^{-1} [average of values given by (102) and (137)]. (49) gives the band oscillator strengths $f_{00} = 2.5 \times 10^{-10}$, $f_{10} \approx 0.2 \times 10^{-10}$. RKR Franck-Condon factors (141)(190); rotational intensity distribution and pressure broadening (100)(102)(137).

^ePressure induced spectra a ← X, b ← X as well as simultaneous transitions in two colliding molecules have been studied by many investigators. See recent papers by (116)(142) which refer to earlier work.

^f(148) give $\nu_{00} = 13122.235 \text{cm}^{-1}$, differing by $+\frac{2}{3}\lambda$ (spin-spin interaction in X $3\Sigma_g^-$) from the zero line of (12).

O₂ (continued):

^gEPR spectra of O₂(¹Δ_g) (62)(126); for ¹⁷O¹⁶O see (132).

^hObserved in absorption in the solar spectrum (10), in emission in a discharge (40) and in the day and twilight glow (29)(45)(91). Values given for the transition probability A₀₀(s⁻¹) are 2.5₈ × 10⁻⁴ (67), 1.9 × 10⁻⁴ (29), 1.5 × 10⁻⁴ (51a). Franck-Condon factors (36)(141)(190); (107).

ⁱω_ey_e = + 0.0474₇, ω_ez_e = - 0.00127₃ (141)(190), see also (5). ΔG($\frac{1}{2}$) = 1556.381 (12)(148)(162), higher ΔG values are less accurately known. G(v) values for v ≤ 28 are listed in (168). RKR potential curve (32)(141)(190).

^jFrom a re-evaluation by (172) of all available microwave and photographic (electronic and Raman) data; these constants supersede earlier results of (144) and are in very good agreement with (180)(181). Spin splitting constants λ₀ = + 1.9847511, γ₀ = - 0.00842536; higher order (centrifugal distortion) constants in (172)(180)(181), see also (165). For v=1, λ₁ = + 1.989586, γ₁ = - 0.0084468 (159), s.
^k+ 0.00006₄₁(v+ $\frac{1}{2}$)² - 2.8₅ × 10⁻⁶(v+ $\frac{1}{2}$)³ (141)(190). | also (154).

B₁ = 1.42192 (148)(159)(168); see also (12).

^lB_v and D_v values for v ≤ 28 are listed in (168).

^mFor microwave data on ¹⁸O₂ see (149), on ¹⁶O¹⁸O (159)(180).

ⁿLaser magnetic resonance spectra (143)(145)(181).

^oThe Stark effect of the 118 GHz fine structure transition (N=1, J=1 ← J=0) has been observed by (163) leading to a reliable value for the polarizability anisotropy α_{||} - α_⊥ = 1.12 Å³.

^pFor Raman data on ¹⁶O¹⁸O and ¹⁸O₂ see (183)(184). The 2-1 hot band was recently resolved in the purely isotropic part of the scattered light (198). Spin structure (130).

(1) Wulf, PNASU 14, 609 (1928).

(2) Hopfield, ApJ 72, 133 (1930).

(3) Childs, Mecke, ZP 68, 344 (1931).

(4) Finkelburg, Steiner, ZP 72, 69 (1932).

(4a) Herzberg, Naturw. 20, 577 (1932).

(5) Curry, Herzberg AP(Leipzig) 19, 800 (1934).

(6) Price, Collins, PR 48, 714 (1935).

(7) Knauss, Ballard, PR 48, 796 (1935).

(8) Herman, AP(Paris) 11, 548 (1939).

(9) Tanaka, Takamine, PR 52, 771 (1941); Sci. Pap. IPGR (Tokyo) 39, 437 (1942).

(10) Herzberg, Herzberg, ApJ 105, 353 (1947).

(11) Kaplan, Nature 159, 673 (1947).

(12) Babcock, Herzberg, ApJ 108, 167 (1948).

(12a) Crawford, Welsh, Locke, PR 75, 1607 (1949).

(13) Feast, PPS A 63, 549 (1950).

(14) Meinel, ApJ 112, 464 (1950); 113, 583 (1951).

(15) Kvifte, Nature 168, 741 (1951).

(16) Herzberg, CJP 30, 185 (1952).

(17) Tanaka, JCP 20, 1728 (1952).

(18) Weissler, Lee, JOSA 42, 200 (1952);
Lee, JOSA 45, 703 (1955).

(19) Herzberg, CJP 31, 657 (1953).

(20) Miller, Townes, PR 90, 537 (1953).

(21) Brix, Herzberg, CJP 32, 110 (1954).

(22) Broida, Gaydon, PRS A 222, 181 (1954).

(23) Aboud, Curtis, Mercure, Rense, JOSA 45, 767 (1955).

(24) Chamberlain, ApJ 121, 277 (1955).

(25) Tinkham, Strandberg, PR 97, 951 (1955).

(26) Barth, Kaplan, JCP 26, 506 (1957); JMS 3, 583 (1959).

(27) Wilkinson, Mulliken, ApJ 125, 594 (1957).

(28) Chamberlain, ApJ 128, 713 (1958).

(29) Vallance Jones, Harrison, JATP 13, 45 (1958).

- O₂: (30) Watanabe, AdGp 5, 153 (1958).
 (30a) Bethke, JCP 31, 669 (1959).
 (31) Carroll, ApJ 129, 794 (1959).
 (32) Vanderslice, Mason, Maisch, JCP 32, 515 (1960).
 (33) Treanor, Wurster, JCP 32, 758 (1960).
 (34) Broida, Peyron, JCP 32, 1068 (1960);
 Schoen, Broida, JCP 32, 1184 (1960).
 (35) Nicholls, CJP 38, 1705 (1960).
 (36) Nicholls, Fraser, Jarman, McEachran, ApJ 131,
 399 (1960).
 (37) Vanderslice, Mason, Maisch, Lippincott, JCP 33,
 614 (1960).
 (38) Weber, McGinnis, JMS 4, 195 (1960).
 (39) Herman, Herman, Rakotoarijimy, JPR 22, 1 (1961).
 (40) Noxon, CJP 39, 1110 (1961).
 (41) Zimmerer, Mizushima, PR 121, 152 (1961).
 (42) Barth, Patapoff, ApJ 136, 1144 (1962).
 (43) Ditchburn, Young, JATP 24, 127 (1962).
 (44) Namioka, Ogawa, Tanaka, Proc. Int. Symp. Mol. Struc-
 ture and Spectroscopy, Tokyo (1962), p. B208-1.
 (45) Noxon, Vallance Jones, Nature 196, 157 (1962).
 (46) Singh, Jain, CJP 40, 520 (1962).
 (47) Nicholson, JCP 39, 954 (1963).
 (48) Dorman, Morrison, JCP 39, 1906 (1963).
 (49) Dianov-Klovov, OS(Engl. Transl.) 16, 224 (1964).
 (50) Jarman, CJP 41, 1926 (1963).
 (51) Krindach, Sobolev, Tunitskii, OS(Engl. Transl.) 15,
 326 (1963).
 (51a) Vallance Jones, Gattinger, PSS 11, 961 (1963).
 (52) Halmann, JCS (1964), 3729.
 (53) Huffman, Larrabee, Tanaka, JCP 40, 356 (1964).
 (54) Cook, Metzger, JCP 41, 321 (1964).
 (55) Jarman, Nicholls. PPS 84, 417 (1964).
 (56) Marr, CJP 42, 382 (1964).
 (57) Ory, Gittleman, ApJ 132, 357 (1964).
 (58) de Reilhac, Damany-Astoin, CR 258, 519 (1964).
 (58a) Bass, Broida, JMS 12, 221 (1964).
 (59) Wacks, JCP 41, 930 (1964).
 (60) Al-Joboury, May, Turner, JCS (1965), 616.
 (61) Halmann, Laulicht, JCP 42, 137 (1965).
 (62) Falick, Mahan, Myers, JCP 42, 1837 (1965).
 (63) Gilmore, JQSRT 5, 369 (1965).
 (63a) Schnepf, Dressler, JCP 42, 2482 (1965).
 (64) Ginter, Battino, JCP 42, 3222 (1965).
 (65) Codling, Madden, JCP 42, 3935 (1965).
 (66) Halmann, Laulicht, JCP 43, 1503 (1965).
 (67) Badger, Wright, Whitlock, JCP 43, 4345 (1965).
 (68) Kosinskaya, Startsev, OS(Engl. Transl.) 18, 416 (1965).
 (69) Blake, Carver, Haddad, JQSRT 6, 451 (1966).
 (70) Degen, Nicholls, JGR 71, 3781 (1966).
 (71) Goldstein, Mastrup, JOSA 56, 765 (1966).
 (72) Turner, May, JCP 45, 471 (1966).
 (73) McNeal, Cook, JCP 45, 3469 (1966).
 (74) Ogawa, SL 15, 97 (1966).
 (75) Samson, Cairns, JOSA 56, 769 (1966).
 (75a) Shapiro, Gush, CJP 44, 949 (1966).
 (76) West, Mizushima, PR 143, 31 (1966).
 (77) Halmann, Laulicht, JCP 46, 2684 (1967).
 (78) Hébert, Innanen, Nicholls, IAMS 4 (1967).
 (79) Huffman, Larrabee, Tanaka, JCP 46, 2213 (1967).
 (80) Jarman, Nicholls, PPS 90, 545 (1967).
 (81) Leclercq, AAP 30, 93 (1967).
 (82) Matsunaga, Watanabe, SL 16, 31 (1967).
 (83) Oppenheim, Goldman, JCP 46, 3493 (1967).
 (84) Alberti, Ashby, Douglas, CJP 46, 337 (1968).
 (85) Ben-Aryeh, JOSA 58, 679 (1968).

- O₂: (86) Ogawa, CJP 46, 312 (1968).
 (87) Degen, CJP 46, 783, 2850 (erratum) (1968).
 (88) Degen, Nicholls, JP B 1, 983 (1968).
 (89) Degen, Innanen, Hébert, Nicholls, IAMS 6 (1968).
 (90) Farmer, Fabian, Lewis, Lokan, Haddad, JQSRT 8, 1739
 (91) Gattinger, CJP 46, 1613 (1968). (1968).
 (92) Hudson, Carter, JOSA 58, 1621 (1968).
 (93) Lindholm, AF 40, 117 (1968).
 (94) McKnight, Gordy, PRL 21, 1787 (1968).
 (95) Myers, Bartle, JCP 48, 3935 (1968).
 (96) Ogawa, Chang, SL 17, 45 (1968).
 (97) Turner, PRS A 307, 15 (1968).
 (98) Yoshino, Tanaka, JCP 48, 4859 (1968).
 (99) Geiger, Schröder, JCP 49, 740 (1968).
 (100) Burch, Gryvnak, AO 8, 1493 (1969).
 (101) Riess, Ben-Aryeh, JQSRT 9, 1463 (1969).
 (102) Miller, Boese, Giver, JQSRT 9, 1507 (1969); 14,
 793 (1974); 16, 595 (1976).
 (103) Buttrey, JQSRT 9, 1527 (1969).
 (104) Degen, Nicholls, JP B 2, 1240 (1969).
 (105) Gebbie, Burroughs, Bird, PRS A 310, 579 (1969).
 (106) Harris, Blackledge, Generosa, JMS 30, 506 (1969).
 (107) Haslett, Fehsenfeld, JGR 74, 1878 (1969).
 (108) Huffman, Larrabee, Baisley, JCP 50, 4594 (1969).
 (109) Albritton, Schmeltekopf, Zare, JCP 51, 1667 (1969).
 (110) Murrell, Taylor, MP 16, 609 (1969).
 (111) Ogawa, Yamawaki, CJP 47, 1805 (1969).
 (112) Siegbahn, Nordling, Johansson, Hedman, Hedén, Hamrin,
 Gelius, Bergmark, Werme, Manne, Baer, "ESCA Applied to
 Free Molecules", North-Holland (1969).
 (113) Ackerman, Biaumé, Kockarts, PSS 18, 1639 (1970).
 (114) Child, JMS 33, 487 (1970).
 (114a) Clark, Wayne, JGR 75, 699 (1970); MP 18, 523 (1970).
 (115) Ackerman, Biaumé, JMS 35, 73 (1970).
 (115a) Boursey, Roncin, Damany, CPL 5, 584 (1970).
 (116) Findlay, CJP 48, 2107 (1970).
 (117) Hasson, Hébert, Nicholls, JP B 3, 1188 (1970).
 (118) Ogawa, JCP 53, 3754 (1970).
 (119) Snopko, OS(Engl. Transl.) 29, 445 (1970).
 (120) Wilheit, Barrett, PR A 1, 213 (1970).
 (121) Allison, Dalgarno, Pasachoff, PSS 19, 1463 (1971).
 (122) Wray, Fried, JQSRT 11, 1171 (1971).
 (123) Bahr, Blake, Carver, Gardner, Kumar, JQSRT 11, 1853
 (1971).
 (124) Butcher, Willetts, Jones, PRS A 324, 231 (1971).
 (125) Durmaz, Murrell, MP 21, 209 (1971).
 (126) Miller, JCP 54, 330 (1971).
 (127) Ogawa, JCP 54, 2550 (1971).
 (128) Freund, JCP 54, 3125 (1971).
 (129) Hasson, Nicholls, JP B 4, 1778, 1789 (1971).
 (130) Rich, Lepard, JMS 38, 549 (1971).
 (131) Sharma, Wray, JCP 54, 4578 (1971).
 (132) Arrington, Falick, Myers, JCP 55, 909 (1971).
 (133) Nakamura, Morioka, Hayaishi, Ishiguro, Sasanuma,
 3rd International Conference on Vacuum Ultraviolet
 Radiation Physics, Tokyo (1971), p. 1pA1-6.
 (134) Schaefer, Miller, JCP 55, 4107 (1971).
 (135) Bergeman, Wofsy, CPL 15, 104 (1972).
 (136) Chang, Ogawa, JMS 44, 405 (1972).
 (137) Galkin, Zhukova, Mitrofanova, OS(Engl. Transl.) 33,
 462 (1972).
 (138) Gerber, HPA 45, 655 (1972).
 (139) Hudson, Mahle, JGR 77, 2902 (1972).
 (140) Jarmain, JQSRT 12, 603 (1972).

- 0₂' (141) Krupenie, JPCRD 1, 423 (1972).
 (142) McKellar, Rich, Welsh, CJP 50, 1 (1972).
 (143) Mizushima, Wells, Evenson, Welch, PRL 29, 831 (1972).
 (144) Welch, Mizushima, PR A 5, 2692 (1972).
 (145) Evenson, Mizushima, PR A 6, 2197 (1972).
 (146) Yamawaki, Ogawa, Internal Technical Report
 University of Southern California Vac-UV-130 (1972).
 (147) Albritton, Harrop, Schmeltekopf, Zare, JMS 46, 25
 (1973).
 (148) Albritton, Harrop, Schmeltekopf, Zare, JMS 46, 103
 (1973).
 (149) Steinbach, Gordy, PR A 8, 1753 (1973).
 (150) Cartwright, Hunt, Williams, Trajmar, Goddard, PR A 8,
 2436 (1973).
 (151) Chang, Ogawa, Internal Technical Report
 University of Southern California Vac-UV-140 (1973).
 (152) Collins, Husain, Donovan, JCS FT II 69, 145 (1973).
 (153) Cook, Ogawa, Carlson, JGR 78, 1663 (1973).
 (154) Cook, Zegarski, Breckenridge, Miller, JCP 58, 1548
 (1973).
 (155) Kinsinger, Taylor, IJMSIP 11, 461 (1973).
 (156) Lee, Carlson, Judge, Ogawa, JQSRT 13, 1023 (1973).
 (157) Tanaka, Tanaka, JCP 59, 5042 (1973).
 (158) Watson, Lang, Stewart, PL A 44, 293 (1973).
 (159) Amano, Hirota, JMS 53, 346 (1974).
 (160) Carbonneau, Marmet, PR A 9, 1898 (1974).
 (161) Carlson, JCP 60, 2350 (1974).
 (162) Fletcher, Rayside, JRS 2, 3 (1974).
 (163) Gustafson, Gordy, PL A 49, 161 (1974).
 (164) Lee, Carlson, Judge, Ogawa, JCP 61, 3261 (1974).
 (165) Veseth, Lofthus, MP 27, 511 (1974).
 (166) Wight, Brion, JESRP 4, 313 (1974).
 (167) Buenker, Peyerimhoff, CP 8, 324; CPL 34, 225 (1975).
 (168) Creek, Nicholls, PRS A 341, 517 (1975).
 (169) Katayama, Huffman, Tanaka, JCP 62, 2939 (1975).
 (170) Dehmer, Chupka, JCP 62, 4525 (1975).
 (171) Huebner, Celotta, Mielczarek, Kuyatt, JCP 63, 241
 (1975).
 (172) Johns, Lepard, JMS 55, 374 (1975).
 (173) Ogawa, Yamawaki, Hashizume, Tanaka, JMS 55, 425 (1975).
 (174) Julianne, Krauss, JMS 56, 270 (1975).
 (175) LaVilla, JCP 63, 2733 (1975).
 (176) Moss, Goddard, JCP 63, 3523 (1975).
 (177) Ogawa, Ogawa, CJP 53, 1845 (1975).
 (178) Samson, Gardner, CJP 53, 1948 (1975).
 (179) Ogawa, CJP 53, 2703 (1975).
 (180) Steinbach, Gordy, PR A 11, 729 (1975).
 (181) Tomuta, Mizushima, Howard, Evenson, PR A 12, 974
 (1975).
 (182) Beebe, Thulstrup, Andersen, JCP 64, 2080 (1976).
 (183) Edwards, Good, Long, JCS FT II 72, 865 (1976).
 (184) Harney, Milanovich, CJS 21, 162 (1976).
 (185) Julianne, JMS 63, 60 (1976).
 (186) Yoshimine, Tanaka, Tatewaki, Obara, Sasaki, Ohno,
 JCP 64, 2254 (1976).
 (187) Julianne, Neumann, Krauss, JCP 64, 2990 (1976).
 (188) Richards, Johnson, JCP 65, 3948 (1976).
 (189) Wraight, Nature 263, 310 (1976).
 (190) Albritton, Schmeltekopf, Zare, "Diatomic Intensity
 Factors", Harper and Row (to be published).
 (191) Lawrence, Barth, Argabright, Science 195, 573 (1977).
 (192) Trajmar, Cartwright, Hall, JCP 65, 5275 (1976).
 (193) Stone, Lawrence, Fairchild, JCP 65, 5083 (1976).
 (194) Buenker, Peyerimhoff, Perić, CPL 42, 383 (1976).

- O_2 : (195) See ref. (29) of O_2^+ . | (1976).
 (196) Cartwright, Fiamengo, Williams, Trajmar, JP B 2, L419
 (197) Fugol, Gimpelevich, Timchenko, OS(Engl. Transl.) 40, 159
 (198) Altmann, Klöckner, Strey, CPL 46, 461 (1977). | (1976).

O_2^+ (continued from p. 505):

- been re-evaluated from more precise measurements by (48)
 who also give improved Λ -type doubling constants.
 $c' + 0.03 \times 10^{-6} (v + \frac{1}{2}) + \dots$; D_v computed from RKR potential (34).
- (1) Bozóky, ZP 104, 275 (1937).
 - (2) Nevin, PTRSL A 237, 471 (1938); PRS A 174, 371 (1940).
 - (3) Nevin, Murphy, PRIA A 46, 169 (1941).
 - (4) Branscomb, PR 72, 619 (1950).
 - (5) Feast, PPS A 63, 557 (1950).
 - (6) Nicolet, Dogniaux, JGR 55, 21 (1950).
 - (7) Vegard, Nature 165, 1012 (1950); AGEP 6, 157 (1950).
 - (8) Dahlstrom, Hunten, PR 84, 378 (1951).
 - (9) Budó, Kovács, APH 4, 273 (1954).
 - (10) Herman, Ferguson, Nicholls, CJP 32, 476 (1961).
 - (10a) Weniger, JPR 23, 225 (1962).
 - (11) Kovács, Weniger, JPR 23, 377 (1962).
 - (12) LeBlanc, JCP 38, 487 (1963).
 - (13) Dorman, Morrison, JCP 32, 1906 (1963).
 - (14) Rao, PPS 81, 240 (1963).
 - (15) Rao, Nature 201, 1112 (1964).
 - (16) Halmann, Laulicht, JCP 43, 1503 (1965).
 - (17) Dufay, Druetta, Eidelsberg, CR 260, 1123 (1965).
 - (17a) Jeunehomme, JCP 44, 4253 (1966).
 - (18) Turner, May, JCP 45, 471 (1966).
 - (19) Spohr, von Puttkamer, ZN 22 a, 705 (1967).
 - (20) Bhale, Rao, PIAS A 67, 350 (1968).
 - (21) Doolittle, Schoen, Schubert, JCP 42, 5108 (1968).
 - (22) Fink, Welge, ZN 23 a, 358 (1968).
 - (23) Nishimura, JPSJ 24, 130 (1968).
 - (24) Dixon, Hull, CPL 2, 367 (1969).
 - (25) Asundi, Ramachandrarao, CPL 4, 89 (1969).
 - (26) Lindholm, AF 40, 117 (1969).
 - (27) See ref. (112) of O_2 .
 - (27a) Albritton, Schmeltekopf, Zare, JCP 51, 1667 (1969).
 - (28) Borst, Zipf, PR A 1, 1410 (1970).
 - (29) Edqvist, Lindholm, Selin, Åsbrink, PS 1, 25 (1970).
 - (30) Jonathan, Morris, Ross, Smith, JCP 54, 4954 (1971).
 - (31) Bhale, JMS 43, 171 (1972).
 - (32) Krupenie, JPCRD 1, 423 (1972).
 - (33) Zare, in "Molecular Spectroscopy: Modern Research", ed. Rao and Mathews, Academic Press (1972), p. 207.
 - (34) Albritton, Harrop, Schmeltekopf, Zare, JMS 46, 89
 - (35) Fairbairn, JCP 60, 521 (1974). | (1973).
 - (36) Gardner, Samson, JCP 61, 5472 (1974).
 - (37) Jonathan, Morris, Okuda, Ross, Smith, JCS FT II 70,
 - (38) Schopman, Loch, CPL 26, 596 (1974). | 1810 (1974).
 - (39) Stockdale, Deleanu, CPL 28, 588 (1974).
 - (40) Gardner, Samson, CPL 32, 315 (1975).
 - (41) Raftery, Richards, JCP 62, 3184 (1975).
 - (42) Gardner, Samson, JCP 62, 4460 (1975).
 - (43) LaVilla, JCP 63, 2733 (1975).
 - (44) Ogawa, Ogawa, JMS 55, 56 (1975).
 - (45) Rao, Kota, Rao, Rao, CS 44, 877 (1975).
 - (46) Veseth, PS 12, 125 (1975).
 - (47) Beebe, Thulstrup, Andersen, JCP 64, 2080 (1976).
 - (48) Colbourn, Douglas, JMS 65, 332 (1977).
 - (49) See ref. (190) of O_2 .
 - (50) Bhale, Narasimham, Pramāṇa 7, 324 (1976).
 - (51) Tabché-Fouhaillé, Durup, Moseley, Ozenne, Pernot, Tadjeddine, CP 17, 81 (1976); PRL 37, 891 (1976).
 - (52) See ref. (3) of O_2^{++} .

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{16}\text{O}_2^+$											
$\mu = 7.9973203_7$ $D_0^0 = 6.663 \text{ eV}^a$ I.P. = 24.2 eV^b										MAR 1977 A	
A detailed review of O_2^+ and its spectrum may be found in (32). Predicted electronic states and potential functions (47); contains references to earlier theoretical work.											
$x_2 \ ^2\Sigma^-$	532.1 eV	} Removal of a $1s_0$ electron from the ground state of O_2 . ^c						$x_2 \rightarrow A,$	526.4 eV ^d	(43)	
$x_1 \ ^4\Sigma^-$	531.0 eV							$x_1 \rightarrow a,$			
								$(x_2 \rightarrow X),$	531.8 eV ^e	(43)	
Several additional states observed in ESCA studies (27) and tentatively assigned by (37).											
$(^2\Sigma_g^-)$	29.5 eV	} Removal of a $2\sigma_g$ electron from the ground state of O_2 . ^f									
$(^4\Sigma_g^-)$	27.5 eV										
$(^2\Sigma_u^-)$	15.8 eV	Removal of a $2\sigma_u$ electron from the ground state of O_2 . ^g									
c $^4\Sigma_u^-$	(100914)	[1545] ^h		[1.561] ⁱ		[6.7]	[1.162 ₀]	c \rightarrow b, V	51540.7 Z	(12)(44)*	
								Hopfield b.			
$(^2\Pi_u)$	(90000)	Diffuse (predissociating) state observed in the photoelectron spectrum of O_2 ; vertical I.P. $\approx 24 \text{ eV}$ (29)(42). Probably highest $^2\Pi_u$ state of configuration $\dots\pi_u^3\pi_g^2$ (24).									
B $^2\Sigma_g^-$	66719	1156 ^j	22 ^j				(1.29 ₈) ^k				
D $(^2\Delta_g)$	62730	920 ^l	(12)				(1.33) ^m				
C $(^2\phi_u)$	(53620)	(900) ⁿ									
b $^4\Sigma_g^-$	49552	1196.77	Z 17.09	0	1.2872 ₉ ^p	0.02206	5.81 ^q	1.2796 ₄	b ^r \rightarrow a, ^s V	16666.74 Z	
								1st negative b.		(2)(3)(10a)	
b' $(^4\Pi_g)$	(48000)	Weakly bound state arising from $^3P + ^4S$ (47); in its unstable region observed by laser photofragment spectroscopy.						b' \leftarrow a,	(51)		
A $^2\Pi_u$	40669.3 ^t	898.2 ₅	Z 13.57 ₃	0	1.0617 ₀	0.0193 ₆ ^u	5.94 ^v	1.4090 ₅	A ^w \rightarrow X, ^x R	40068.1 Z	
								2nd negative b.		(1)(5)(20) (32)(34)(48) (50)	
a $^4\Pi_{ui}$	32964 ^y	1035.69	Z 10.39	0	1.1046 ₆	0.01575 ^z	4.88 ^z	1.3813 ₈			
x $^2\Pi_g$	197.3 ^{a'} 0	1904.7 ₇	Z 16.25 ₉	0	1.6913	0.01976 ^{b'}	5.32 ^{c'}	1.1164			

O_2^+ : $a_D^0(O_2) + I.P.(O) - I.P.(O_2)$.

b From the electron impact appearance potential of O_2^{++} , A.P. = 36.3 eV (13), and I.P.(O_2). (52) give A.P. = 37.2 eV.

c Highly excited states (K limits) observed in X-ray photoelectron (27) and emission (43) spectra.

d Unresolved vertical transitions.

e Predicted vertical transition; in the X-ray emission spectrum of (43) this transition is hidden by an artefact.

f Observed in the low-resolution X-ray photoelectron spectrum of (27). In the 304 Å photoelectron spectrum (40)(42) find a very broad maximum corresponding to $4\Sigma_g^-$ and two sharp peaks (I.P. 40.33 and 40.40 eV) corresponding to $2\Sigma_g^-$.

g Observed in the X-ray PE spectrum (27). A very weak broad maximum appears near 27.5 eV in the 304 Å PE spectrum of (29); not confirmed by (42). See also (37).

h Average of values obtained by PE spectroscopy (29) and from the limits of Codling and Madden's Rydberg series.

i Spin splitting constant $\epsilon = 0.44 \text{ cm}^{-1}$. Only bands having $v'=0$ occur in emission; predissociation (29)(38).

j From the limits of Tanaka and Takamine's Rydberg series; in good agreement with constants obtained from PE spectra (29). Predissociation (21)(38)(39).

k Franck-Condon factor analysis of PE band intensities (37).

l Only observed in the PE spectrum of $O_2(^1\Delta_g)$ (30)(37); tentatively identified as convergence limit of a fragmentary Rydberg series (26). Predissociation (38).

m Franck-Condon factor analysis of the PE spectrum (37).

n Only observed in the PE spectrum of $O_2(^1\Delta_g)$ (37); vibrational numbering uncertain.

o RKR potential curves (32)(49). Calculated Franck-Condon factors for ionizing transitions from $X^3\Sigma_g^-, a^1\Delta_g, b^1\Sigma_g^+$ (16)(25)(32)(49), and for recombination transitions from $X^2\Pi_g$ and $a^4\Pi_u$ to $B^3\Sigma_u^-$ (32). (16) give also results for

$16_0^{18}O$ and $18_0^{18}O$; note, however, that their calculations for transitions to $X^2\Pi_g$ are based on the previously accepted but now abandoned vibrational numbering for the ground state of O_2^+ and lead to disagreement with observed photoelectron intensities (19). Experimental Franck-Condon factors from photoelectron spectra (29)(36)(42).

p Spin splitting constant $\epsilon = 0.1487 \text{ cm}^{-1}$.

q $\beta_e = +0.185 \times 10^{-6}$.

r Radiative lifetime $\tau = 1.15 \mu\text{s}$ (17a)(22)(28)(35).

s Observed in various discharges (14) and in aurorae (6)(7)(8)(15). Excitation by electron impact (23), by fast ions (10)(17). Franck-Condon factors (32)(49). Rotational line strengths (33).

t A_v increases from $A_0 = -3.6$ to $A_{15} = +10.0$ (31)(34)(48)(50). Theoretical interpretation (41).

u $r_e = -0.000173$; constants fitted to $v' \leq 8$ (34). Additional B_v values up to $v=15$ are listed by (48) who also give Λ -type doubling constants.

$v + 0.06(v+\frac{1}{2}) + 0.012(v+\frac{1}{2})^2$; the D_v values have been computed (34) from the experimental potential curve.

w Radiative lifetime $\tau = 0.69 \mu\text{s}$ (17a)(22).

x Excitation by electron impact; its effect on the rotational temperature (4). Franck-Condon factors (25)(27a)(32)(49).

y $A_0 \dots A_6 = -47.79 \dots -48.01$ (11); anomalous dependence on J of the multiplet splitting (9)(11). T_e calculated from the limit ($b^4\Sigma_g^-$) of Tanaka and Takamine's Rydberg series with I.P.(O_2), $v_{00}(b \rightarrow a)$, and the constants for a, X .

z Constants representing $v=0, 1, 2$; $\beta_e = -0.095 \times 10^{-6}$ (2). For $v=3 \dots 6$ see (3)(10a). Slightly different constants in (46).

a' A_v decreases from $A_0 = +200.33$ (48) to $A_{10} = +192.05$ (34). See also (41).

b' Constants fitted to $v \leq 10$ (34). Selected B_v values have (continued on p. 503)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
<div><div><div><div><div>$^{16}\text{O}_2^{++}$</div></div></div><div><div><div>c</div><div>94000</div></div><div>b</div><div>54000</div></div><div>a ($^3\Sigma_u^+$)</div><div>32500</div></div><div>x $^1\Sigma_g^+$</div><div>0</div></div> <div>}</div> <div><div>$\mu = 7.9971832_2$</div><div><u>Ab initio</u> predicted electronic states and potential curves (7); empirical calculations of spectroscopic constants (1).</div><div>Additional states observed by Auger electron spectroscopy (4).</div><div>Detected by double charge transfer spectroscopy [$\text{H}^+ + \text{O}_2 \rightarrow \text{H}^- + \text{O}_2^{++}$] (5).</div><div>Observed in electron impact experiments (3) and in the Auger electron spectrum (4).</div><div>Locally stable, observed by electron impact mass-spectrometry (2)(3)(6).</div></div>											MAR 1977
<div><div><div><div><div>$^{16}\text{O}_2^-$</div></div></div><div><div><div>b</div><div>118540</div></div><div>a ($^4\Pi_u$)</div><div>97800</div></div><div>A ($^2\Pi_u$)</div><div>(25300)</div></div><div>x $^2\Pi_{gi}$</div><div>0^j</div></div> <div><div>$\mu = 7.9975946_6$</div><div>$D_0^0 = 4.094_4 \text{ eV}^a$</div><div>I.P. = 0.440 eV^b</div><div>1290</div><div>1044</div><div>10</div><div>Short progression of resonances in electron transmission.^c</div><div>Long progression of resonances in electron transmission.^e</div><div>Additional resonances in the electron transmission current at 8-11 eV^d.</div><div>Several bound excited states predicted by theoretical calculations (12).</div><div>(574.5)^g</div><div>(7.1)^g</div><div>Photodetachment cross sections 6700 - 4600 \AA ($14900 - 21800 \text{ cm}^{-1}$).</div><div>1090^k</div><div>8.1^k</div><div>1.35^l</div><div>$A \leftrightarrow X$,^h</div><div>(25000)ⁱ</div><div>Raman sp.^m</div><div>EPR sp.ⁿ</div></div> <div><div>14.27 eV^d</div><div>11.68 eV^f</div><div>(1a)(11)</div><div>(15)</div><div>(1b)(3)</div><div>(1)(2a)</div></div>											MAR 1977

- O_2^{++} : (1) Hurley, JMS 2, 18 (1962).
 (2) Dorman, Morrison, JCP 39, 1906 (1963).
 (3) Daly, Powell, PPS 90, 629 (1967).
 (4) Moddeman, Carlson, Krause, Pullen, Bull, Schweitzer, JCP 55, 2317 (1971).
 (5) Appell, Durup, Fehsenfeld, Fournier, JP B 6, 197 (1973).
 (6) Meyerson, Ihrig, IJMSIP 10, 497 (1973).
 (7) Beebe, Thulstrup, Andersen, JCP 64, 2080 (1976).

- O_2^- : ^aFrom $D_0^0(O_2)$ and the electron affinities of O (1.462 eV) and O_2 .
^bFrom the O_2^- photodetachment spectrum (9); see also (2). From endothermic negative-ion charge-transfer reactions (6) obtain I.P. $\geq 0.45 \pm 0.1$ eV. The theoretical value is 0.42 eV (10).
^c"Band b". Suggested "grandparent" state $b^4\Sigma_g^-$ of O_2^+ .
^dEnergy relative to $X^3\Sigma_g^-(v=0)$ of neutral O_2 .
^e"Band a". The negative ion state results from the addition of two Rydberg electrons in the $3s\sigma_g$ orbital to the O_2^+ core in the $a^4\Pi_u$ state ("grandparent").
^fExtrapolated energy of $v=0$ relative to $X^3\Sigma_g^-(v=0)$ of neutral O_2 .
^gAbsorption in KBr, vibrational numbering uncertain (11).
^hObserved in alkali halide crystals at 4.2 and 2 K.
ⁱEstimated ν_{00} for the free O_2^- ion, by extrapolation from data for various host crystals (3).
^j $A = -160 \text{ cm}^{-1}$ (13).
^kFrom electron scattering cross sections for gaseous O_2 (4)(5); similar measurements by (7) suggest $w_e = 1140$, $w_e x_e = 12$. A direct measurement of $\Delta G(\frac{1}{2})$ in the photodetachment spectrum (9) gives $\sim 1090 \text{ cm}^{-1}$, in agreement with extrapolations from Raman frequencies in alkali

O_2^- (continued):

halide crystals (3). Anharmonicities derived from low-temperature fluorescence spectra (see ^h) are approximately 8.7 (11).

^lFrom a Franck-Condon factor analysis of the photodetachment spectrum (9) and a similar evaluation by (16) of the electron scattering data of (5).

^mIn alkali halide crystals and in solid KO_2 and NaO_2 .

ⁿIn alkali halide crystals.

- (1) Känzig, Cohen, PRL 3, 509 (1959).
 (1a) Rolfe, JCP 40, 1664 (1964).
 (1b) Creighton, Lippincott, JCP 40, 1779 (1964).
 (2) Pack, Phelps, JCP 44, 1870 (1966).
 (2a) Zeller, Känzig, HPA 40, 845 (1967).
 (3) Rolfe, Holzer, Murphy, Bernstein, JCP 49, 963 (1968); JMS 26, 543 (1968).
 (4) Boness, Schulz, PR A 2, 2182 (1970).
 (5) Linder, Schmidt, ZN 26 a, 1617 (1971).
 (6) Tiernan, Hughes, Lifshitz, JCP 55, 5692 (1971).
 (7) Gray, Haselton, Krause, Soltysik, CPL 13, 51 (1972).
 (8) Sanche, Schulz, PR A 6, 69 (1972).
 (9) Celotta, Bennett, Hall, Siegel, Levine, PR A 6, 631 (1972).
 (10) Zemke, Das, Wahl, CPL 14, 310 (1972).
 (11) Ikezawa, Rolfe, JCP 58, 2024 (1973).
 (12) Krauss, Neumann, Wahl, Das, Zemke, PR A 7, 69 (1973).
 (13) Land, Raith, PRL 30, 193 (1973).
 (14) Schulz, RMP 45, 423 (1973).
 (15) Cosby, Ling, Peterson, Moseley, JCP 65, 5267 (1976).
 (16) Parlant, Fiquet-Fayard, JP B 2, 1617 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{16}\text{O}^1\text{H}$		$\mu = 0.94808710$ $D_0^0 = 4.392 \text{ eV}^a$ I.P. = 12.9_0 eV^b Theoretical potential functions for 48 states (92); for $X^2\Pi$ and $A^2\Sigma^+$ see (112)(113)(118). Strong many-line spectrum 1900-1700 \AA , tentative identification.								MAY 1977 A
C $^2\Sigma^+$	89459.1	1232.9	Z 19.1	4.247 ^{cd}	0.078	2	2.046 ₁	$C^e \rightarrow A,^m R$	55820.7 Z	(20)(42)(64)*
D $^2\Sigma^-$	(82130)	(2954)		[15.2179] ^f		[16.16]	[1.0809 ₃]	$(C \rightarrow X)^e$	(88223)	(20)(46)*
B $^2\Sigma^+$	69774	[660.0]	Z i	[5.086] ^{jd}	k	[9.29] ^l	[1.869 ₈]	$D \leftarrow X,^g R$	81759.7 ^h Z	(106)
A $^2\Sigma^+$	32684.1	3178.8 ₆	Z 92.91 ₇ ⁿ	17.358 ^{opqd}	0.786 ₈ ^r	[20.39] ^s	1.0121	$B \rightarrow A,^m R$	35965.5 Z	(16)(20)(33) (42)* (58)* (64)* (73)
X $^2\Pi_1$	0 ^v	3737.76 ₁	Z 84.881 ₃ ^w	18.910 ₈ ^{xd}	0.7242 ^y	19.38 ^z	0.96966	$A^t \leftrightarrow X,^u R$	32402.3 ^h Z	(3)(57)(64)*
								$\frac{1}{2} \leftarrow \frac{3}{2} a'$	126.23	(69a)(90)
								Rotation - vibr. b. b'c'		
								1-0 sequence		(18)(27)(122)
								2-0 sequence		(8)(27)(29) (122)
								3-0 sequence		(36)(122)
								4-0 sequence		(10)(11)(14) (36)
								other sequences		(11)(14)(26) (36)
								Rotation sp.		(13)(107) (124)
								Hf Λ -doubling sp. ^{d'e'f'}		(12)(41)(60) (105)(115) (117)(126)
								EPR sp. ^{g'}		(35)(69)(72) (78)(93)(109)

^0H : ^aShort extrapolation of the vibrational levels in $A^2\Sigma^+$, assuming that this state has no potential maximum; confirmed by the observed predissociation in $B^2\Sigma^+$ (64). $D_e = 4.621 \text{ eV}$, in complete agreement with the most recent theoretical value (121).

^bPhotoionization mass-spectrometry of HOF (99); 13.01 eV from the photoelectron

^cSpin splitting constants $\gamma_0 \dots \gamma_3 = +1.09 \dots +0.67$ (20)(64). | spectrum (125).

^dRKR potential functions (32)(66).

^eLifetime of the upper state of the $C \rightarrow A$ system $\sim 6 \text{ ns}$; measurements in the 1700-1900 \AA region give $\tau \approx 2 \text{ ns}$ which, in spite of the poor agreement, is not inconsistent with the assignment of at least part of these bands to $C \rightarrow X$ (120). Much longer lifetimes ($\sim 80 \text{ ns}$) have been reported by (83).

^fSpin splitting constant $\gamma_0 = -0.293$.

^gTheoretical oscillator strength $f_{00} = 0.0036$ (119).

O^1H : ^aShort extrapolation of the vibrational levels in $A^2\Sigma^+$, assuming that this state has no potential maximum; confirmed by the observed predissociation in $B^2\Sigma^+$ (64). $D_e = 4.621 \text{ eV}$, in complete agreement with the most recent theoretical value (121).

^bPhotoionization mass-spectrometry of HOF (99); 13.01 eV from the photoelectron spectrum (125).

^cSpin splitting constants $\gamma_0 \dots \gamma_3 = +1.09 \dots +0.67$ (20)(64). | spectrum (125).

^dRKR potential functions (32)(66).

^eLifetime of the upper state of the $C \rightarrow A$ system $\sim 6 \text{ ns}$; measurements in the 1700-1900 \AA region give $\tau \approx 2 \text{ ns}$ which, in spite of the poor agreement, is not inconsistent with the assignment of at least part of these bands to $C \rightarrow X$ (120). Much longer lifetimes ($\sim 80 \text{ ns}$) have been reported by (83).

^fSpin splitting constant $\gamma_0 = -0.293$.

^gTheoretical oscillator strength $f_{00} = 0.0036$ (119).

^hEnergy of $N'=0$ relative to the zero-point of the Hill-Van Vleck expression for the ground state.

ⁱUsing isotope relations (16) estimates $w_e = 940$, $w_e x_e = 105$, $w_e y_e = -21.5$.

^jSpin splitting const. $\gamma < 0.03$ (64). Prediss. by rotation in $v=0$ above $N=15$, in $v=1$ above $N=9$; diss. products $^1S + ^2S$ (42)(64).

O^1H (continued):

^k $B_1 = 4.119$. Constants for the B state are from (64).

^l $D_1 = 29.1 \times 10^{-4}$, $H_1 = -15 \times 10^{-5}$.

^mFranck-Condon factors (42).

ⁿ $-1.791_5(v+\frac{1}{2})^3 + 0.3236_2(v+\frac{1}{2})^4 - 0.03585(v+\frac{1}{2})^5$ (16). Energy levels and improved $\Delta G(v+\frac{1}{2})$ values are listed in (64).

^oSpin splitting constants $\gamma_0 \dots \gamma_3 = 0.201, 0.196, 0.192, 0.193$ (79); see also (3).

^pPredissociation in $v=0$ above $N=23$, in $v=1$ above $N=14$, and of all levels in $v=2$; from the lifetime measurements of (89)(98)(116). A sharp decrease in the intensity of emission lines originating from the predissociated levels has been observed at or slightly above threshold in low pressure flames and discharges (5)(9)(55); (21) report corresponding intensity increases due to inverse predissociation in hydrogen flames; see also (63). The predissociation is noticeably stronger for the F_1 than for the F_2 levels; according to (59)(67)(75)(98)(101)(111)(116) it is caused by the $^4\Sigma^-$ state arising from $^3P + ^2S$, but the possibility of predissociation by the $^2\Pi$ ground state has also been considered (74)(77). A much stronger predissociation of $A \ ^2\Sigma^+$ leading to diffuseness in the $B \rightarrow A$ bands has been observed (20)(58)(64) for $v=5, 6, 7$ at all N levels and for $v=8$ above $N=6$; according to (73) it is produced by the $^4\Pi$ state arising from $^3P + ^2S$.

^q $\mu_{el}(v=0) = 1.98$ D from high-field Stark effects on the $A \rightarrow X$ transition (84).

^r $\gamma_e = -0.016$. The equilibrium constants were derived by (16) to fit B_v from $v=0$ to 4. Improved B_v values ($v=0 \dots 3$) have been obtained by (79) from the data of (3); additional B_v values for $v \leq 9$ are listed in (16)(20)(42)(64). For term values ($v=0 \dots 3$) see (79).

^sOther D_v values in (79) and (16)(20)(42)(64); $H_0 = 8.7_1 \times 10^{-8}$ (79).

^tRadiative lifetimes $\tau(v=0, N=1) = 693 \pm 10$ ns, $\tau(v=1, N=1) = 736 \pm 11$ ns (116). The increase from $v=0$ to $v=1$ and a similar variation with increasing rotation in $v=0$ [(116), see also (89)(98)] are explained by the dependence on r of the transition moment [see (116) and references given there]. (108) using a method very similar to (116) obtain 720 and 765 ns for the average lifetimes of several low-lying rotational levels in $v=0$ and 1, respectively. Earlier apparently less accurate determinations (89)(91)(98)(103)(104) gave somewhat higher τ values [see also (45)]; Hanle effect measurements (86)(100) are slightly lower. The decay time of the predissociated $v=2$ level (see ^p) is 203 ± 13 ns for $N=0$ and decreases rapidly at higher N (116); estimated non-radiative lifetime for $N=1 \sim 270$ ns. High-resolution line absorption measurements by (96) [see also (44)] give $f_{00} = 0.00095$ for the rotationless molecule in reasonable agreement with lifetime measurements but in sharp contrast to $f_{00} = 0.0014_8$ obtained by (50) using the hook method; f_{10} values are, respectively, 0.00024 and 0.0008₉.

^uObserved in emission in all kinds of electric discharges (often as an impurity), in flames (34) and in the heads of comets; in absorption in H_2O vapour at high temperature (1) and in electric discharges (2), in flames (28), in the flash photolysis of H_2O , $O_3 + H_2O$, and other mixtures (31)(37)(53), and in stellar spectra, especially the solar spectrum (24). Emission and absorption in solid neon (61). Atlas of $A-X$ bands (7), new measurements of the 0-0 and 1-0 bands (87). Magnetic rotation spectrum (82). Franck- (continued on p. 510)

O^1H (continued):

Condon factors (17)(25)(42). Vibrational intensity distribution (3)(114); rotational intensity distribution (39)(54); effect of variation of transition moment with r and dependence on J (51)(114).

$$^vA_v = -139.21 - 0.275v \quad (122).$$

$^w + 0.5409(v+\frac{1}{2})^3 - 0.02134(v+\frac{1}{2})^4 - 0.00113(v+\frac{1}{2})^5$, representing the vibrational levels up to $v=5$ (122); see also (10)(11).

$$\Delta G(\frac{1}{2}) = 3569.64_0 \quad (122).$$

$^x\Lambda$ -type doubling parameters $p_v = 0.235 - 0.006v$, $q_v = -0.0391 + 0.0018v$, see (122) who give also centrifugal distortion terms. See y .

$^y + 0.00706(v+\frac{1}{2})^2 - 0.00050(v+\frac{1}{2})^3$, representing $B_0 \dots B_5$ (122); slightly different constants in (10)(79)(85)(90). Term values for $v \leq 3$ tabulated in (3)(79), for $v=4,5,6$ in (10), for $v=7,8,9$ in (36).

$$^z - 0.432 \times 10^{-4}(v+\frac{1}{2}) + 0.024 \times 10^{-4}(v+\frac{1}{2})^2; H_0 = 14.2 \times 10^{-8} \quad (122). \text{ See } ^y.$$

a The 79 μm electric dipole spectrum ($^2\Pi_{\frac{1}{2}}, J=\frac{1}{2} \leftarrow ^2\Pi_{\frac{3}{2}}, J=\frac{3}{2}$) has been measured by the laser magnetic resonance method.

b Observed in emission in the spectrum of the night sky (4)(11)(15)(22)(26), in the $\text{H} + \text{O}_3$ reaction (14)(19)(36)(81), in the $\text{H} + \text{O}_2$ reaction (27), and in oxyacetylene flames (8)(18)(29)(122). In absorption in rare gas matrices (62).

c Radiative lifetimes derived from observed intensities: $\tau(v=1) = 24 \text{ ms}$, $\tau(v=2) = 12 \text{ ms}$ (97); from the decay rate of the $9 \rightarrow 7$ radiation: $\tau(v=9) = 64 \text{ ms}$ (80). The dipole moment function has been studied by many authors, most recently by (38)(76)(81) and (97) from measured band strengths and transition probabilities. An extensive ab initio calculation of the dipole moment function is given by (112) [see also (113)]. (110) has used this ab initio

function to predict absolute intensities of a large array of vibration-rotation transitions taking account of spin uncoupling and vibration-rotation interaction [see also the early work of (6) and (40)].

d The 18 cm transition ($^2\Pi_{3/2}, J=3/2$) consists of four components (23)(47a)(88):

$F'=1 \leftarrow F''=2$	1612.2310 ₁ MHz
$F'=1 \leftarrow F''=1$	1665.4018 ₄ MHz
$F'=2 \leftarrow F''=2$	1667.3590 ₃ MHz
$F'=2 \leftarrow F''=1$	1720.5299 ₈ MHz

Einstein A coefficients for these transitions have been calculated by (49). Calculated frequencies for ^{17}OH (102).

e Hfs and Λ -doubling constants. From Stark shifts of the hf Λ -doubling transitions (48)(95) determine $\mu_{e\ell}(v=0) = 1.6676 \text{ D}$.

f Also observed in interstellar clouds, see the reviews in (52)(56)(65). In some clouds there is strong evidence for maser action. In the laboratory population inversion between Λ -doublet states was recently observed by (123).

g Observed in $v=0 \dots 9$. Hyperfine and Λ -doubling constants. EPR spectrum of ^{17}OH (68).

- (1) Bonnhoeffer, Reichardt, ZPC A 139, 75 (1928).
- (2) Oldenberg, JCP 3, 266 (1935).
- (3) Dieke, Crosswhite, Bumblebee Series Report No. 87, Johns Hopkins University (1948); JQSRT 2, 97 (1962).
- (4) Meinel, ApJ 111, 555 (1950).
- (5) Gaydon, Wolfhard, PRS A 208, 63 (1951).
- (6) Heaps, Herzberg, ZP 133, 48 (1952).
- (7) Bass, Broida, NBS Circular 541 (1953).
- (8) Benedict, Plyler, Humphreys, JCP 21, 398 (1953).
- (9) Broida, Kane, PR 89, 1053 (1953).

- O^1H : (10) Herman, Hornbeck, ApJ 118, 214 (1953).
 (11) Chamberlain, Roesler, ApJ 121, 541 (1955).
 (12) Dousmanis, Sanders, Townes, PR 100, 1735 (1955).
 (13) Madden, Benedict, JCP 23, 408 (1955).
 (14) McKinley, Garvin, Boudart, JCP 23, 784 (1955).
 (15) Vallance Jones, Nature 175, 950 (1955).
 (16) Barrow, AF 11, 281 (1956).
 (17) Nicholls, PPS A 69, 741 (1956).
 (18) Allen, Blaine, Plyler, SA 2, 126 (1957).
 (19) Kraus, ZN 12 a, 479 (1957).
 (20) Michel, ZN 12 a, 887 (1957).
 (21) Charton, Gaydon, PRS A 245, 84 (1958).
 (22) Connes, Gush, JPR 20, 915 (1959).
 (23) Ehrenstein, Townes, Stevenson, PRL 3, 40 (1959).
 (24) Moore, Broida, JRNBS A 63, 279 (1959).
 (25) Nicholls, Fraser, Jarman, CF 3, 13 (1959).
 (26) Blackwell, Ingham, Rundle, ApJ 131, 15 (1960).
 (27) Charters, Polanyi, CJC 38, 1742 (1960).
 (28) Gaydon, Spokes, van Suchtelen, PRS A 256, 323 (1960).
 (29) Rogge, Yarger, Dickey, JCP 33, 453 (1960).
 (30) Wallace, ApJ 132, 894 (1960).
 (31) Basco, Norrish, PRS A 260, 293 (1961).
 (32) Fallon, Tobias, Vanderslice, JCP 34, 167 (1961).
 (33) Herman, Felenbok, Herman, JPR 22, 83 (1961).
 (34) Krishnamachari, Broida, JCP 34, 1709 (1961).
 (35) Radford, PR 122, 114 (1961); 126, 1035 (1962).
 (36) Bass, Garvin, JMS 2, 114 (1962).
 (37) Black, Porter, PRS A 266, 185 (1962).
 (38) Ferguson, Parkinson, PSS 11, 149 (1963).
 (39) Learner, PRS A 269, 311 (1962).
 (40) Cashion, JMS 10, 182 (1963).
 (41) Ehrenstein, PR 130, 669 (1963).
 (42) Felenbok, AAP 26, 393 (1963).
 (43) Kayama, JCP 39, 1507 (1963).
 (44) Golden, del Greco, Kaufman, JCP 39, 3034 (1963).
 (45) Bennett, Dalby, JCP 40, 1414 (1964).
 (46) Felenbok, Czarny, AAP 27, 244 (1964).
 (47) Phelps, Dalby, CJP 43, 144 (1964).
 (47a) Radford, PRL 13, 534 (1964).
 (48) Powell, Lide, JCP 42, 4201 (1965).
 (49) Turner, Nature 212, 184 (1966); 214, 379 (1967).
 (50) Anketell, Pery-Thorne, PRS A 301, 343 (1967).
 (51) Anketell, Learner, PRS A 301, 355 (1967).
 (52) Barrett, Science 157, 881 (1967).
 (53) Horne, Norrish, Nature 215, 1373 (1967).
 (54) Meinel, ZN 22 a, 977 (1967).
 (55) Naegeli, Palmer, JMS 23, 44 (1967); 28, 417 (1968).
 (56) Robinson, McGee, ARAA 5, 183 (1967).
 (57) Stoebner, Delbourgo, JCPPB 64, 1115 (1967).
 (58) Czarny, Felenbok, AAP 31, 141 (1968).
 (59) Palmer, Naegeli, JMS 28, 417 (1968).
 (60) Poynter, Beaudet, PRL 21, 305 (1968).
 (61) Tinti, JCP 48, 1459 (1968).
 (62) Acquista, Schoen, Lide, JCP 48, 1534 (1968).
 (63) Gutman, Lutz, Jacobs, Hardwidge, Schott, JCP 48, 5689
 (64) Carlone, Dalby, CJP 47, 1945 (1969). | (1968).
 (65) Cook, Physica 41, 1 (1969).
 (66) Horsley, Richards, JCPPB 66, 41 (1969).
 (67) Michels, Harris, CPL 3, 441 (1969).
 (68) Carrington, Lucas, PRS A 314, 567 (1970).
 (69) Churg, Levy, ApJ 162, L161 (1970).
 (69a) Evenson, Wells, Radford, PRL 25, 199 (1970).
 (70) Smith, JCP 53, 792 (1970).
 (71) Veseth, JP B 3, 1677 (1970).

- O¹H:
- (72) Clough, Curran, Thrush, PRS A 323, 541 (1971).
 - (73) Czarny, Felenbok, Lefebvre-Brion, JP B 4, 124 (1971).
 - (74) Durmaz, Murrell, TFS 62, 3395 (1971).
 - (75) Gaydon, Kopp, JP B 4, 752 (1971).
 - (76) d'Incan, Effantin, Roux, JQSRT 11, 1215 (1971);
12, 97 (1972).
 - (77) Julianne, Krauss, Donn, ApJ 170, 65 (1971).
 - (78) Lee, Tam, Larouche, Woonton, CJP 49, 2207 (1971).
 - (79) Moore, Richards, PS 3, 223 (1971).
 - (80) Potter, Coltharp, Worley, JCP 54, 992 (1971).
 - (81) Murphy, JCP 54, 4852 (1971).
 - (82) Nanes, Robinson, JCP 55, 963 (1971).
 - (83) Remy, SpL 4, 319 (1971).
 - (84) Scarl, Dalby, CJP 49, 2825 (1971).
 - (85) Veseth, JMS 38, 228 (1971).
 - (86) de Zafra, Marshall, Metcalf, PR A 3, 1557 (1971).
 - (87) Engleman, JQSRT 12, 1347 (1972).
 - (88) ter Meulen, Dymanus, ApJ 172, L21 (1972).
 - (89) Elmergreen, Smith, ApJ 178, 557 (1972).
 - (90) Mizushima, PR A 5, 143 (1972).
 - (91) Becker, Haaks, ZN 28 a, 249 (1973).
 - (92) Easson, Pryce, CJP 51, 518 (1973).
 - (93) Hinkley, Walker, Richards, PRS A 331, 553 (1973).
 - (94) Klein, JQSRT 13, 581 (1973).
 - (95) Meerts, Dymanus, CPL 23, 45 (1973).
 - (96) Rouse, Engleman, JQSRT 13, 1503 (1973).
 - (97) Roux, d'Incan, Cerny, ApJ 186, 1141 (1973).
 - (98) Sutherland, Anderson, JCP 58, 1226 (1973);
59, 6690 (1973) (erratum).
 - (99) Berkowitz, Appelman, Chupka, JCP 58, 1950 (1973).
 - (100) German, Bergeman, Weinstock, Zare, JCP 58, 4304
(1973).
 - (101) Palmer, Naegeli, JCP 59, 994 (1973).
 - (102) Valtz, Soglasnova, ApL 13, 23 (1973).
 - (103) Becker, Haaks, Tatarczyk, CPL 25, 564 (1974).
 - (104) Brophy, Silver, Kinsey, CPL 28, 418 (1974).
 - (105) Destombes, Marlière, Rohart, Burie, Journal,
CR B 278, 275 (1974); 280, 809 (1975).
 - (106) Douglas, CJP 52, 318 (1974).
 - (107) Ducas, Javan, JCP 60, 1677 (1974).
 - (108) Hogan, Davis, CPL 29, 555 (1974).
 - (109) Lee, Tam, CP 4, 434 (1974).
 - (110) Mies, JMS 53, 150 (1974).
 - (111) Smith, Elmergreen, Brooks, JCP 61, 2793 (1974).
 - (112) Stevens, Das, Wahl, Krauss, Neumann, JCP 61, 3686
(1974).
 - (113) Chu, Yoshimine, Liu, JCP 61, 5389 (1974).
 - (114) Crosley, Lengel, JQSRT 15, 579 (1975).
 - (115) Destombes, Marlière, CPL 34, 532 (1975).
 - (116) German, JCP 62, 2584; 63, 5252 (1975).
 - (117) Meerts, Dymanus, CJP 53, 2123 (1975).
 - (118) Meyer, Rosmus, JCP 63, 2356 (1975).
 - (119) Ray, Kelly, ApJ 202, L57 (1975).
 - (120) Smith, Stella, JCP 63, 2395 (1975).
 - (121) Arnold, Whiting, Sharbaugh, JCP 64, 3251 (1976).
 - (122) Maillard, Chauville, Mantz, JMS 63, 120 (1976).
 - (123) ter Meulen, Meerts, van Mierlo, Dymanus, PRL 36,
1031 (1976).
 - (124) Downey, Robinson, Smith, JCP 66, 1685 (1977).
 - (125) Katsumata, Lloyd, CPL 45, 519 (1977).
 - (126) Meerts, CPL 46, 24 (1977).

O²H (continued from p. 515):

- (18) de Zafra, Marshall, Metcalf, PR A 3, 1557 (1971).
- (19) Elmergreen, Smith, ApJ 178, 557 (1972).
- (20) Becker, Haaks, ZN 28 a, 249 (1973).
- (21) Clyne, Coxon, Woon Fat, JMS 46, 146 (1973).
- (22) German, Bergeman, Weinstock, Zare, JCP 58, 4304 (1973).
- (23) Meerts, Dymanus, ApJ 180, L93 (1973).
- (24) Meerts, Dymanus, CPL 23, 45 (1973).
- (25) Rouse, Engleman, JQSRT 13, 1503 (1973).
- (26) Weinstock, Zare, JCP 58, 4319 (1973).
- (27) Brophy, Silver, Kinsey, CPL 28, 418 (1974).
- (28) Carlone, PR A 2, 606 (1974).

- (29) Douglas, CJP 52, 318 (1974).
- (30) Carlone, PR A 12, 2464 (1975).
- (31) Coxon, JMS 58, 1 (1975).
- (32) Coxon, Hammersley, JMS 58, 29 (1975).
- (33) German, JCP 62, 2584; 63, 5252 (1975).
- (34) Meerts, Dymanus, CJP 53, 2123 (1975).
- (35) Smith, Stella, JCP 63, 2395 (1975).
- (36) Wilcox, Anderson, Peacher, JOSA 65, 1368 (1975).
- (37) German, JCP 64, 4192 (1976).
- (38) Woods, Dixon, JCP 64, 5319 (1976).
- (39) Crosley, Lengel, JQSRT 17, 59 (1977).
- (40) Katsumata, Lloyd, CPL 45, 519 (1977).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{16}\text{O}^2\text{H}$		$\mu = 1.78884797$ $D_0^0 = 4.453 \text{ eV}^a$ I.P. = 12.9_1 eV^b								MAY 1977
C $^2\Sigma^+$	(89470)	(898)	(10)	[2.235] ^c			[2.053]	$\text{C}^d \rightarrow \text{A},^e \text{R}$	56090.3 Z	(7)(13)*
		Strong many-line spectrum 1900-1700 \AA , tentative identification.						$(\text{C} \rightarrow \text{X})^d$	(88568)	(8)*
D $^2\Sigma^-$	(82160)	(2074)		[8.2283] ^f		[5.179]	[1.0701 ₈]	$\text{D} \leftarrow \text{X}, \text{R}$	81853.22 ^g Z	(29)
B $^2\Sigma^+$	69775	[546.9]	Z h	[2.745] ⁱ	j	[2.50] ^k	[1.852 ₉]	$\text{B} \rightarrow \text{A},^l \text{R}$	36275.7 Z	(5)(6)(7)* (9)(13)*
A $^2\Sigma^+$	32680.8 ₅ ^m	2316.17	Z 50.433 ⁿ	9.193 ₆ ^{opqr}	0.318 ₁ ^s	[5.763] ^t	1.0124	$\text{A}^u \leftrightarrow \text{X},^v \text{R}$	32477.18 ^g Z	(13)* (21) (31)
X $^2\Pi_i$	0 ^w	2720.24	Z 44.055	10.020 ₉ ^{xr}	0.275 ₇ ^y	[5.374] ^z	0.9697 ₅	Hf Λ -doubling sp. ^{a'} EPR sp. ^{b'}		(4)(23)(34) (14)

O^2H : ^aFrom $D_0^0(\text{O}^1\text{H})$ assuming zero electronic isotope shift.
^bFrom I.P. (O^1H) and the zero-point energies of OH, OD, OH⁺, OD⁺. Photoelectron spectroscopy gives 13.01 eV (40).
^cSpin splitting constant $\gamma_0 = +0.6$.
^dLifetimes of 6.1 and ~ 2 ns have been reported (35) for the upper state of the C \rightarrow A bands and for the 1850 \AA group, respectively. See ^e of O^1H .
^eOnly the 0-11 and 0-12 bands have been observed (13).
^fSpin splitting constant $\gamma_0 = -0.156$.
^gSee ^h of O^1H .
^h $\Delta G(3/2) = 357.9$ (13). Using isotope relations (5) derives $w_e = 684$, $w_e x_e = 55.7$, $w_e y_e = -8.3$.
ⁱSpin splitting constant $\gamma < 0.05$.
^j $B_1 = 2.445$, $B_2 = 1.947$ (13).
^k $D_1 = 4.48 \times 10^{-4}$, $D_2 = 18.9 \times 10^{-4}$; $H_0 = -12 \times 10^{-7}$, $H_1 = -16 \times 10^{-7}$ (13).
^lFranck-Condon factors (7).

^m T_e has been corrected for the effects of Y_{00} on the zero-point energy in both upper and lower state and for a small electronic term σ_V^Σ due to interaction with the $^2\Pi$ state; see (31).
ⁿ $w_e y_e = -0.2350$; the constants represent only $v=0\dots 3$ (31). Vibrational energy levels and ΔG values up to $v=13$ are listed in (13). Preliminary vibrational constants may be found in (5).
^oSpin splitting constants (31): $\gamma_0 = +0.1201$ [good agreement with (29)], $\gamma_1 = +0.117_0$, $\gamma_2 = +0.111_4$.
^pIn low-pressure flames and discharges the intensity of emission lines originating in $v'=0,1,2$ decreases rapidly above $N'=29,26,17$, respectively (3), owing to predissociation by $^4\Sigma^-$ (see ^p of O^1H); substantially higher N' values in (10) correspond to the first lines of zero intensity. The lifetime of the $v'=0$ rotational levels drops sharply above $N'\approx 34$ (19)(36). A much stronger predissociation

O^2H (continued):

occurs for $v=7\dots 12$ causing diffuseness in the $B \rightarrow A$ bands in low pressure discharges (13)(15); asymmetric line shapes in the 0-9 band have been studied by (28) and have been found (30) to contain a Q component because of mixing with the $^4\Pi$ state that causes the predissociation (15).

$q_{el}(v=0) = 2.16 \text{ D}$ (17), see q of O^1H . A considerably lower value of 1.72 D was derived by (26) from Stark shifts in the location of high-field level crossings and appears to be favoured by ab initio calculations [for references see (26)]. Hfs constants from high-field level crossing experiments in (26) [eqQ corrected by (38)] and (37).

r_{RKR} potential functions (31).

$s_e^y = -0.00119$. The equilibrium constants refer to the true mechanical B_v values derived by (31) from the effective constants (given in the same paper) for $v \leq 3$. Term values for $v \leq 3$ (21).

$t + 1.65 \times 10^{-8} J^3(J+1)^3 - 6.0 \times 10^{-13} J^4(J+1)^4$ (31); good agreement with D_0 and H_0 of (29). (31) gives D_v , H_v for $v \leq 2$.

u Radiative lifetimes $\tau(v=0, N=1) = 691 \pm 9 \text{ ns}$, $\tau(v=1, N=1) = 712 \pm 10 \text{ ns}$, $\tau(v=2, N=1) = 736 \pm 13 \text{ ns}$ (33). (19)(20)(27) (36) give somewhat longer lifetimes for low rotational levels in $v=0$; Hanle effect measurements (18)(22) are slightly lower. Oscillator strengths from high-resolution line absorption: $f_{00} = 0.00096$ and $f_{10} = 0.00026$ for the rotationless molecule (25).

v Zeeman effect in the 0-0 band (12)(16), magnetic rotation spectrum (16). Absorption and emission in solid Ne (11). Franck-Condon factors (7)(31). Vibrational intensity distribution, variation of the transition moment with r , rotational dependence of transition probabilities (39).

w $A_0 = -139.23_0$, $A_1 = -139.44_0$, $A_2 = -139.64_4$ (31). Ab

initio calculation of spin-orbit coupling parameters (32).

x Λ -type doubling parameters $p_0 = +0.1266$, $q_0 = -0.01093_4$; additional constants for $v \leq 3$ (31); ab initio calc. (32).

y $r_e = +0.000_6$. Term values for $v \leq 3$ (21).

z $D_1 = 5.331 \times 10^{-4}$, $D_2 = 5.28 \times 10^{-4}$; $H_0 = +1.93_5 \times 10^{-8}$, $H_1 = +2.06_5 \times 10^{-8}$, $H_2 = +2.46 \times 10^{-8}$; $L_0 = -5.2 \times 10^{-13}$ (31). For $v=0$ good agreement with (29).

a Λ -doubling and hfs coupling constants. Dipole moment $\mu_{el}(v=0) = 1.6531_2 \text{ D}$, from Stark shifts of hf Λ -doubling transitions (24); see also (17).

b Spectrum of ^{17}O D; magnetic hf and electric quadrupole coupling constants.

- (1) Sastry, IJP 15, 95, 455 (1941); 16, 27, 169, 343 (1942); Sastry, Rao, IJP 15, 27 (1941).
- (2) Oura, JPSJ 6, 401 (1951); LTS 6, 41 (1951).
- (3) Broida, Kane, PR 89, 1053 (1953).
- (4) Dousmanis, Sanders, Townes, PR 100, 1735 (1955).
- (5) Barrow, AF 11, 281 (1956).
- (6) Herman, Felenbok, Herman, JPR 2, 83 (1961).
- (7) Felenbok, AAP 26, 393 (1963).
- (8) Felenbok, Czarny, AAP 27, 244 (1964).
- (9) Czarny, Felenbok, AAP 31, 141 (1968).
- (10) Palmer, Naegeli, JMS 28, 417 (1968).
- (11) Tinti, JCP 48, 1459 (1968).
- (12) Thakur, Rai, Singh, JCP 48, 3389 (1968).
- (13) Carlone, Dalby, CJP 47, 1945 (1969).
- (14) Carrington, Lucas, PRS A 314, 567 (1970).
- (15) Czarny, Felenbok, Lefebvre-Brion, JP B 4, 124 (1971).
- (16) Nanes, Robinson, JCP 55, 963 (1971).
- (17) Scarl, Dalby, CJP 49, 2825 (1971).

(continued on p. 513)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{16}\text{O}^1\text{H}^+$										
$D_0^0 = 5.0_9 \text{ eV}^a$										
b $1\Sigma^+$ (29050)	[2981] ^b			[16.320] ^b	(0.732) ^b	[19.2] ^b	1.032	(b-X)	29058.8 ^b	MAY 1977
A $3\Pi_1 \begin{Bmatrix} 0^+ \\ 1 \\ 2 \end{Bmatrix}$ 28438.55	2133.65	Z	79.55	13.791 ₆ ^{cd}	0.8889 ^e	[22.49 ₅] ^f	1.1354	$A^g \rightarrow X, {}^h R \begin{Bmatrix} 28034.04^i \\ 28028.31^i \\ 27948.43^i \\ 27864.31^i \end{Bmatrix}$	(2)* n	
a 1Δ 17660 ^j										
X $3\Sigma^-$ 0	3113.37	Z	78.52	16.794 ₃ ^k	0.7494 ^l	[19.17 ₄] ^m	1.0289			
$^{16}\text{O}^2\text{H}^+$										
$D_0^0 = 5.1_4 \text{ eV}^o$										
b $1\Sigma^+$ (29050)	[2174] ^b			[8.736 ₉] ^b	(0.285) ^b	[5.44] ^b	1.030	(b-X)	29051.2 ^b	MAY 1977
A $3\Pi_1 \begin{Bmatrix} 0^+ \\ 1 \\ 2 \end{Bmatrix}$ 28452.75	1558.08	Z	44.438 ^p	7.310 ₇ ^{qr}	0.3398 ^s	[6.38 ₈] ^t	1.1354	$A^u \rightarrow X, {}^h R \begin{Bmatrix} 28181.47^i \\ 28176.06^i \\ 28095.83^i \\ 28011.57^i \end{Bmatrix}$	(2)* n	
a 1Δ 17660 ^j				$B_6 = 7.242_4^v$		v				
X $3\Sigma^-$ 0	2271.80	Z	44.235 ^w	8.911 ₆ ^x	0.2896 ^y	[5.44] ^z	1.0283			
$^{16}\text{O}^1\text{H}^-$										
$D_0^0 = 4.755 \text{ eV}^a$ I.P. = 1.825 ₄ eV ^b										
a (3Π) (28000)	Absorption ($\lambda < 3500 \text{ \AA}$) and long-lived emission ($\lambda_{\text{max}} \approx 4000 \text{ \AA}$) in aqueous solutions.									
X $1\Sigma^+$ 0	(3700) ^c			(18.9) ^c			(0.970) ^c			(3)
$^{16}\text{O}^2\text{H}^-$										
$D_0^0 = 4.814 \text{ eV}^d$ I.P. = 1.823 ₀ eV ^b										
X $1\Sigma^+$ 0	(2700) ^c			(10.02) ^c			(0.970) ^c			
(^{192}Os)^{16}O ?										
$(\mu = 14.7646702_7)$										
Mostly R shaded emission bands in the region 11400 - 16400 cm^{-1} . No analysis.										
APR 1975										
(1)* (2)										

0^1H^+ , 0^2H^+ ,

^a $D_0^0(0^1H) + I.P.(H) - I.P.(0^1H)$.

^bConstants derived from the perturbations in $A^3\Pi$. The b-X transition is not observed.

^c Λ -doubling constants $p_0 = -0.251$, $q_0 = +0.0478$; for $v=1,2$ see (2).

^dPerturbations by b $1\Sigma^+$.

^e $\gamma_e = +0.0173_0$.

^f $H_0 = +10.4 \times 10^{-8}$; other D_v , H_v values for $v \leq 2$ in (2).

^gLifetime $\tau(v=0) = 0.89 \mu s$ (1); similar results for $v=1,3$.

^hVibrational intensity distribution (branching ratios), variation of the transition moment with r (3).

ⁱSubband origins as defined by (2). From the data for the $OD^+ A^3\Pi(v=0)$ level (2) estimate the true spin-orbit and spin-spin interaction parameters $A = -83.83 \text{ cm}^{-1}$ and $2\alpha = -5.9_2 \text{ cm}^{-1}$.

^jFrom the photoelectron spectrum (4).

^kSpin splitting constants for $v=0$: $\lambda_0 = 2.13_4 \text{ cm}^{-1}$ and $\gamma_0 = -0.147_8 \text{ cm}^{-1}$; similar results for $v=1$ and 2.

^l $\gamma_e = +0.0109_7$.

^m $H_0 = +12.3_9 \times 10^{-8}$; values for D_1 , D_2 in (2).

ⁿA rather complete list and critical assessment of earlier references is given in (2).

^oFrom $D_0^0(0^1H^+)$.

^p $w_e \gamma_e = +0.368_3$.

^q Λ -doubling constants $p_0 = -0.132$, $q_0 = +0.0122_2 \text{ cm}^{-1}$; for $v=1,2,3$ see (2).

^rPerturbations by b $1\Sigma^+$ and a 1Δ .

^s $\gamma_e = +0.00372$.

^t $H_0 = +2.0_2 \times 10^{-8}$; other D_v , H_v values for $v \leq 3$ in (2).

^uLifetime $\tau(v=0) = 1.06 \mu s$ (1a).

^vThis level at 29434 cm^{-1} is only observed through pertur-

0^1H^+ , 0^2H^+ (continued):

bations in $A^3\Pi(v=1)$; $D_6 = 4.8 \times 10^{-4}$. The $v=5$ level produces a weak perturbation in $A^3\Pi(v=0)$.

^w $w_e \gamma_e = +0.426_7$.

^xSpin splitting constants $\lambda_0 = +2.141$, $\gamma_0 = -0.079_0 \text{ cm}^{-1}$; similar constants for $v=1,2$ (2).

^y $\gamma_e = +0.00300$.

^z $H_0 = 2.1_7 \times 10^{-8}$; values for D_1 , D_2 , D_3 in (2).

(1) Brzozowski, Elander, Erman, Lyyra, PS 10, 241 (1974).

(1a) Brzozowski, Erman, Lew, CPL 34, 267 (1975).

(2) Merer, Malm, Martin, Horani, Rostas, CJP 53, 251 (1975).

(3) Gérard, Govers, van de Runstraat, Marx, CPL 44, 154

(4) Katsumata, Lloyd, CPL 45, 519 (1977). | (1976).

0^1H^- , 0^2H^- ,

^aFrom $D_0^0(OH)$ and the electron affinities of OH and O.

^bFrom high-resolution photodetachment studies of OH^- and OD^- (5); see also (1)(2)(4).

^cEstimates based on the analysis of photodetachment data

^dAnalogous to a. | (1)(4)(5).

(1) Branscomb, PR 148, 11 (1966).

(2) Kay, Page, TFS 62, 3081 (1966).

(3) Merkel, Hamill, JCP 55, 2174 (1971).

(4) Celotta, Bennett, Hall, JCP 60, 1740 (1974).

(5) Hotop, Patterson, Lineberger, JCP 60, 1806 (1974).

OsO: (1) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(2) Raziunas, Macur, Katz, JCP 43, 1010 (1965).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	v ₀₀	
³¹ P ₂		μ = 15.4868817		D ₀ ⁰ = 5.033 eV ^a		I.P. = 10.53 eV ^b				MAY 1977 A
		Carroll and Mitchell's Rydberg series V _n converging to F ² Σ _u ⁺ (v=0):								
...4σ _u 5σ _g ² 2π _u ⁴ nsσ _g ^c		v = 125225 - R/(n-1.86) ² , n = 5(V ₅),6...16. Similar series with v'=1.								(21)
v ₅ (¹ Σ _u ⁺)	114085	[789]						V ₅ ← X,	114090	(21)
		Carroll and Mitchell's Rydberg series G _n , H _n , P _n , R _n converging to A ² Σ _g ⁺ (v=0):								
...4σ _u ² 5σ _g ² 2π _u ⁴		v = 87179 - { R/(n-0.062-0.633/n* ²) ² , n = 4(R ₄),5...21. R/(n-0.155+0.179/n* ²) ² , n = 4(P ₄),5...14. R/(n-1.468-0.475/n* ²) ² , n = 4(H),5(H ₅),6...28. R/(n-1.660-0.252/n* ²) ² , n = 4(G),5(N),6(G ₆),7...12.								(21)*
		Carroll and Mitchell's Rydberg series E _n , K _n , M _n , L _n converging to X ₂ ² Π _{1/2} (v=1):								
...4σ _u ² 5σ _g ² 2π _u ³		v ≈ 85895 - { R/(n+0.04) ² , n = 3(L),4. R/(n-0.03) ² , n = 3(M),4(M ₄),5(S). R/(n-0.12) ² , n = 3(K),4...10. R/(n-1.93) ² , n = 4(E),5(E ₅),6.						Fragments of series with v'=0 (v _∞ = 85229) and with v' > 1.		(21)*
		Unclassified bands 79700 - 84500 cm ⁻¹ .								(21)
U	83362	[551]	H	Observed to v'=2.				U← X,	R 83248	H (21)*
G ₆ (¹ Σ _u ⁺)	81327	[723]		Diffuse bands.				G ₆ ← X,	R 81299	H (9)(21)
T	80992	[713.1]	H	Observed to v'=4.				T← X,	R 80958.5	H (9)(21)*
S ¹ Σ _u ⁺	(80840)			B ₁ = 0.2783			r ₁ = 1.978	S← X,	R 81453.89 ^d	Z (9)(21)
R ₄ (¹ Π _u)	80115	[740]		Broad diffuse bands.				R ₄ ← X,	80095	(21)
Q (¹ Π _u)	(79860)	[617.6]	H	0-0 and 1-1 bands only.				Q← X,	R 79779.5 ₃	H (9)(21)
P ₄ (¹ Σ _u ⁺)	(79827)			Broad band.				P ₄ ← X,	79804	(21)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (Å)	Observed Transitions		References	
								Design.	v_{00}		
3^1P_2 (continued)											
$M_4(^1\Sigma_u^+)$	(78271)	(705)	(5)	Only $v'=1$ and 3(diffuse) observed.				$M_4 \leftarrow X$, R	(78233) ^e	(21)	
$H_5(^1\Pi_u)$	(78256)			Very broad band.				$H_5 \leftarrow X$,	78233	(21)	
$K_4(^1\Pi_u)$	(77968)	[732]		Diffuse bands.				$K_4 \leftarrow X$,	77944	(21)	
O	77475	529	H	2				$O \leftarrow X$, R	77349	H (21)*	
N $^1\Sigma_u^+$	77286.7	[641.76]	Z	(29.7)	0.2984 ^f	0.0050 ₄	[3.1]	1.909 ₉	N $\leftarrow X$, R	77240.2 ₃	Z (9)(21)
L $(^1\Pi_u)$	73593	[672.2]	H						L $\leftarrow X$, R	73539.3	H (9)(21)
$E_5(^1\Pi_u)$	73385	685	H	2.7					$E_5 \leftarrow X$, R	73337	(21)
M $^1\Sigma_u^+$	73168.0	684.0 ^g	H	2.9 ₇	0.2802 ^g	0.0016		1.971	M $\leftarrow X$, R	73119.6 ^g	H (9)(21)
K $^1\Pi_u$	72288	[701.7]	H ^Q	(5)	[0.2704] ^{hf}			[2.006]	K $\leftarrow X$, R	72253.3	Z (9)(21)
Numerous diffuse irregularly spaced "lines" 69900 - 70400 cm^{-1} , no assignments.										(9)	
H $(^1\Pi_u)$	(68960)	Very intense diffuse band, width $\sim 80 \text{ cm}^{-1}$.							H $\leftarrow X$,	68940	(9)(21)

P_2 : ^aFrom the predissociation limit in $C^1\Sigma_u^+$ which according to (1) is equal to the dissociation limit $4S + 2D$. The latest thermochemical (mass-spectrometric) value is 5.04 eV (17) eliminating the possibility that the predissociation limit corresponds to $2D + 2D$ as suggested by (16).

^bFrom the photoelectron spectrum (25) which shows partially resolved peaks at 10.53 and 10.55 eV corresponding to $X_1^2\Pi_{3/2}$ and $X_2^2\Pi_{1/2}$, respectively. Subtraction of the estimated doublet splitting in the $X^2\Pi$ ground state [$\sim 260 \text{ cm}^{-1}$, see ref. (6) of P_2^+] from the Rydberg series limit at 85229 cm^{-1} (21) gives 10.53₅ eV.

^cCore configuration as suggested by (25) on the basis of ab initio calculations; Carroll and Mitchell (21) proposed ...4 $\sigma_u^2 5\sigma_g 2\pi_u^3 2\pi_g$.

^dAssigned as 0-0 band by (9), reassigned as 1-0 band by (21) [third member of the $M_n(v'=1)$ Rydberg series].

^e0-0 band obscured by $H_5 \leftarrow X$ 0-0.

^fRKR potential functions (10)(13).

^gFollowing (21) the v' numbering of (9) has been increased by one unit.

^hAll lines of this system are diffuse; the diffuseness is largest for $v'=3$ and 4 such that the rotational structure can no longer be recognized. The broadening is independent of J ; the state causing the predissociation is probably $1\Pi_u$.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^3\text{P}_2$ (continued)										
I $^1\Pi_u$	[68849.3]			[0.2541]		[2.5]	[2.070]	I \leftarrow X, R	68459.6 ₃ Z	(9)
G $^1\Sigma_u^+$	66313.37	694.12 Z	4.18 ₂	0.29730 ^f	0.00195	[2.25]	1.9135	G \leftrightarrow X, R	66269.71 Z	(6)(9)*
E $^1\Pi_u$	59446.21	700.66 H ^q	2.92	[0.2807 ₂] ^f		[1.84]	[1.969 ₂]	E \leftrightarrow X, ⁱ R	59406.14 Z	(6)(9)*
B $^1\Pi_u$	50845.9	[358.96] ^j Z	k	[0.2268] ^j	^l	[3.2]	[2.191]	B \rightarrow A, R	16203.7 ₁ ^j Z	(18)(23)*
c $^3\Pi_u$	² 47176.8 ¹ 47159.1 ⁰ 47139.2	393.67 Z	3.849 ^m	0.2190 ⁿ	0.0024	2.5	2.229	c \rightarrow b, ^o R	18721.5 Z 18836.4 Z 18944.6 Z	(15)(22)* (26)(27) (1)*(2)*(4)
C $^1\Sigma_u^+$	46941.26	473.93 Z	2.340 ^p	0.24211 ^{qf}	0.00175 ^r	2.57	2.1204	C \leftrightarrow X, R	46787.97 Z	(9)(11)* (23)*
A $^1\Pi_g$	34515.25	618.95 Z	3.00	0.27524	0.00168	2.2	1.9887	A \rightarrow X, R	34434.30 Z	(7)* (14) (18)(23)*
b $^3\Pi_g$	² 28329.6 ¹ 28197.0 ⁰ 28068.9	644.66 Z	3.213 ^s	0.2805	0.00178	2.0	1.970	b \rightarrow a, ^o V	9574.8 Z 9442.2 Z 9314.1 Z	(12)(20) (22)* (26)
b' $^3\Sigma_u^-$	28503.4 ^t	604.4 ₈ Z	2.2	0.2584 ^u	0.0014	1.7	2.052	b' \rightarrow X, R	28415.4 Z	(12)(19)*
a $^3\Sigma^+$	18794.5	565.1 ₇ H	2.7 ₅	B ₁ = 0.2503 ₃ ^v	D ₁ = 3.3 x 10 ⁻⁷		r ₁ = 2.085 ₃	(a - X)	18686.7 ^w	
X $^1\Sigma_g^+$	0	780.77 Z	2.83 ₅ ^x	0.30362 ^f	0.00149 ^y	1.88	1.8934			

P_2 (continued):

ⁱFranck-Condon factors (13).

^jThe assignment of $v'=0$ to the lowest observed level is arbitrary.

^k $\Delta G(3/2) = 352.71$.

^lB₁ = 0.2209, B₂ = 0.217₁.

^m $w_{ey_e} = -0.0915$ (26); slightly different constants in (27).

ⁿPerturbations by C $^1\Sigma_u^+$. The observation of extra lines enables the relative position of singlet and triplet levels to be determined (26); very similar results have been obtained by (24)(27).

^oFranck-Condon factors (22).

^p $w_{ey_e} = +0.0066$. Constants from (9), but see (27) whose deperturbation of the C state levels (see ^q) leads to $T_e =$

P₂ (continued):

46945.5₇, $w_e = 472.81$, $w_e x_e = 2.24_6$, $w_e y_e = + 0.00412_2$.
^qStrong vibrational perturbations for $v=1,2,3,5$ (1) and many rotational perturbations (3)(4)(5)(9)(23) due to interaction with levels of $c\ ^3\Pi_u$; see (27). Breaking off in emission (predissociation) above $J=58$ of $v=10$ and $J=34$ of $v=11$; the corresponding dissociation limit is $^4S + ^2D$ at $51959 \pm 25\text{ cm}^{-1}$. A second predissociation indicated by diffuseness in absorption begins at $v=17$ and reaches a maximum for low J values of $v=19$ (9).
^r $y_e = + 3.3 \times 10^{-6}$.
^s $w_e y_e < 0.001\text{ cm}^{-1}$ (26); slightly different constants in (27).
^tRecalculated; (19) give 28507.7₄ which probably refers to data obtained from band heads rather than band origins.
^uSpin splitting constants $\lambda = +3.20$, $\gamma = -0.001$.
^vSpin splitting constants $\lambda_1 = -3.2_1$, $\gamma_1 = -0.003$ (22).
^wNot observed; indirectly derived (26) from perturbations in $c\ ^3\Pi_u$; see ⁿ.
^x $w_e y_e = - 0.00462$ (27); slightly different constants in (4) and (9).
^y $y_e = - 2.7 \times 10^{-6}$. Constants recalculated from the data of (1)(7)(9)(11). Higher B_v values not included in the re-evaluation may be found in (1)(4).

- (1) Herzberg, AP(Leipzig) (5) 15, 677 (1932).
- (2) Ashley, PR 44, 919 (1933).
- (3) Marais, PR 70, 499 (1946).
- (4) Marais, Verleger, PR 80, 429 (1950).
- (5) Naudé, Verleger, PR 80, 432 (1950).
- (6) Dressler, HPA 28, 563 (1955).
- (7) Douglas, Rao, CJP 36, 565 (1958).
- (8) Gutbier, ZN' 16 a, 268 (1961).
- (9) Creutzberg, CJP' 44, 1583 (1966).
- (10) Singh, Rai, IJPAP 4, 102 (1966).
- (11) Dixit, PIAS A 66, 325 (1967).
- (12) Mrozowski, Santaram, JOSA 57, 522 (1967).
- (13) Rao, Lakshman, IJPAP 8, 617 (1970).
- (14) Verma, Broida, CJP 48, 2991 (1970).
- (15) Brion, Da Paz, Mongin, Guenebaut, CR B 272, 999 (1971).
- (16) Vaidyan, Santaram, IJPAP 9, 1022 (1971).
- (17) Kordis, Gingerich, JCP 58, 5141 (1973).
- (18) Malicet, Brion, Guenebaut, CR C 276, 991 (1973).
- (19) Brion, Malicet, Guenebaut, CJP 52, 2143 (1974); 53, 201 (1975) (erratum).
- (20) Brion, Malicet, JP B 8, L164 (1975).
- (21) Carroll, Mitchell, PRS A 342, 93 (1975).
- (22) Brion, Malicet, JP B 9, 2097 (1976).
- (23) Brion, Malicet, Guenebaut, CJP 54, 362 (1976).
- (24) Brion, Malicet, Merienne-Lafore, CR C 283, 171 (1976).
- (25) Bulgin, Dyke, Morris, JCS FT II 72, 2225 (1976).
- (26) Carroll, Nulty, JP B 9, L427 (1976).
- (27) Brion, Malicet, Merienne-Lafore, CJP 55, 68 (1977).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
31P_2^+											
		$\mu = 15.4867445$		$D_0^0 = 4.99 \text{ eV}^a$						MAY 1977	
F ($^2\Sigma_u^+$)	(40180) ^b	[810] ^b									
C ₂ $2\Pi_g$ 3/2	28870.6 ^c	441.47 ^d	Z	2.58	0.2162 ₉	0.00136	2.0	2.243 ₄	C ₂ →X ₁ , R 28754.2 ^d Z	(1)* (2)(6)*	
C ₁ $2\Pi_g$ 1/2	(28686.6)								C ₁ →X ₂ , R 28312.3 ^d Z		
B $2\Sigma_u^+$	(25566)	410.50 ^e	Z	3.23	0.2419 ^e	0.00211	3.3	2.121	B→A, R 23224.8 ₉ ^e Z	(1)*	
D ₂ $2\Pi_g$ 1/2	(18832.5)	462.2		2.45	0.2196	0.00142	2.0	2.226	D ₂ →X ₂ , R 18467.6 Z	(3)(6)*	
D ₁ $2\Pi_g$ 3/2	18740.7								D ₁ →X ₁ , R 18635.8 Z		
A $2\Sigma_g^+$	(2179) ^f	[733.0] ^g Z			0.3037 ^g	0.0021		1.893			
X ₂ $2\Pi_u$ 1/2	(260) ^h	672.20 ^d	Z	2.74	0.2760 ₀	0.00151	2.0	1.985 ₉			
X ₁ $2\Pi_u$ 3/2	0										
$(208)\text{Pb}_2$											
		$(\mu = 103.988329)$		$D_0^0 = 0.8_2 \text{ eV}^a$						MAY 1977 A	
		Emission bands in the region 12500 - 11100 cm^{-1} , observed in Ar and Ne matrices by excitation with argon/krypton ion laser lines.									(7)
		Absorption bands in the regions 33400 - 34600 cm^{-1} (preceded by continuous fluctuations from 31300 to 33300 cm^{-1}), 36800 - 38000, and 41000 - 42200 cm^{-1} .									(2)
B	19490.3	161.64 ^b	H	1.036 ^c					B↔X, ^d R 19515.7 H	(1)* (2)* (4)	
A	14465.6	162.4 ^b		0.4					A↔X, ^e (R) 14491.5	(2)* (4)(5)	
X	0	110.5 ^{bf}	H	0.35							
$(208)\text{Pb}^{209}\text{Bi}$											
		$(\mu = 104.238661)$		$D_0^0 = 1.4_3 \text{ eV}^a$						MAY 1977	

P_2^+ : ^a $D_0^0(P_2) + I.P.(P) - I.P.(P_2)$.

^bFrom Rydberg series of P_2 (4) and observations by photoelectron spectroscopy (5).

^c A_v strongly dependent on v , $A_{v+1} - A_v = -4.13 \text{ cm}^{-1}$ (6).

^dVibrational numbering of (6); the previous numbering of (1) has been increased by one unit in both upper (C) and lower (X) state following the recommendations of (4).

^eVibrational numbering uncertain; the B state has not been observed in the photoelectron spectrum (5).

^fFrom Rydberg limits of P_2 (4) and the estimated spin splitting in the ground state of P_2^+ ; in reasonable agreement with the photoelectron-spectroscopic value of 2230 cm^{-1} (5).

^gVibrational numbering uncertain.

^hThe magnitude of the spin-orbit coupling in the $^2\Pi$ ground and excited states has been estimated (6) from the effective B values. The photoelectron spectrum (5) suggests for the ground state a spin splitting of $\sim 150 \text{ cm}^{-1}$.

(1) Narasimham, CJP 35, 1242 (1957).

(2) Brion, Malicet, Guenebaut, CR C 276, 471 (1973).

(3) Brion, Malicet, Guenebaut, CR C 276, 551 (1973).

(4) Carroll, Mitchell, PRS A 342, 93 (1975).

(5) Bulgin, Dyke, Morris, JCS FT II 72, 2225 (1976).

(6) Malicet, Brion, Guenebaut, CJP 54, 907 (1976).

Pb_2 : ^aThermochemical value (mass-spectrom.) (6).

^bConstants obtained by (4) from a reclassification of bands in the blue-green and in the red system. The new analysis of the ground state seems to be confirmed by the observation of a lower state frequency of 111 cm^{-1} in laser-excited matrix emission spectra [see (7) who attribute the 111 cm^{-1} interval to a matrix-induced splitting of the ground state]. The revised lower state constants imply, however, a strong contradiction to the usual rule that if $\omega' > \omega''$ then $B' > B''$ since according to the published spectrograms of (2) the B-X bands are strongly shaded to the red, i.e. $B' < B''$.

^c $\omega_{e,y_e} = + 0.0055$.

^dPreviously called A-X. Also observed in inert gas matrices (3)(7).

^ePreviously believed to have B as its lower state.

^f(4) give 119.1 which seems to be a typographical or arithmetical error since it does not represent the band head measurements of (1).

(1) Shawhan, PR 48, 343 (1935).

(2) Weniger, JP(Paris) 28, 595 (1967).

(3) Brewer, Chang, JCP 56, 1728 (1972).

(4) Johnson, Cannell, Lunacek, Broida, JCP 56, 5723 (1972).

(5) Puri, Mohan, IJPAP 13, 206 (1975).

(6) Gingerich, Cocke, Miller, JCP 64, 4027 (1976).

(7) Teichman, Nixon, JMS 52, 299 (1976).

$PbBi$: ^aThermochemical value (mass-spectrom.) (1).

(1) Rovner, Drowart, Drowart, TFS 63, 2906 (1967).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(208)Pb⁷⁹Br										
		$(\mu = 57.209681_3)$		$D_0^0 = (2.5) \text{ eV}^a$		$\text{I.P.} = 7.8 \text{ eV}^b$				JUL 1977
B ($^2\Sigma$)	34523.7	258.2	H 0.60	Diffuse bands (prediss.)				B \leftarrow X ₁ , V	34549.0	H (2)*
A ($\frac{1}{2}$)	20884.3	152.5	H 0.40 ^c	d				A \leftrightarrow X ₁ , R	20856.8	H (1)(3)(6)
X ₁ $^2\Pi_{1/2}$	0	207.5	H 0.50 ^e	d						
(208)Pb³⁵Cl										
		$(\mu = 29.9355409)$		$D_0^0 = (3.1) \text{ eV}^a$		$\text{I.P.} = 7.5_5 \text{ eV}^b$				JUL 1977
B ($^2\Sigma$)	35199 ^c	382.1 ^c	H 1.05 ^c	Diffuse bands (prediss.)				B \leftarrow X ₁ , V	35238 ^c	H (3)*
A ($\frac{1}{2}$)	21865.0	228.7	H 0.78	d				A \rightarrow X ₂ , R	13546.2	H (5)
X ₂ $^2\Pi_{3/2}$	8272.2	321.6	H 0.3 ^e					A \leftrightarrow X ₁ , R	21827.4	H (1)(2)* (5)* (8)
X ₁ $^2\Pi_{1/2}$	0	303.9	H 0.88	d						
208Pb¹⁹F										
		$\mu = 17.4081886$		$D_0^0 = 3.6_4 \text{ eV}^a$		$\text{I.P.} = 7.5 \text{ eV}^b$				JUL 1977
Strong absorption continuum with maximum at $\sim 41000 \text{ cm}^{-1}$; emission continuum with maximum at $\sim 32800 \text{ cm}^{-1}$.										
F	(47866)	[628]	H					F \leftarrow X ₁ , (V)	47927	H (2)
E	(45400)	(565)	H					E \rightarrow X ₂ , V		(5)
D	(43818)	[597]	H					E \leftarrow X ₁ , V	45430	H (2)
C	38046	594.0	H 2.50	Diffuse bands ^c				D \leftarrow X ₁ , (V)	43863	H (2)
B $^2\Sigma^+$	35644.4	[605.75]	Z 3.42 H ^Q	0.24810 ^{de}	0.001479	1.63	1.9756	C \leftarrow X ₁ , V	38089	H (2)
								B \leftrightarrow X ₂ , V	27420.91	Z (2)* (7)* (8)
								B \leftrightarrow X ₁ , V	35696.79	Z (2)* (8)
A $\frac{1}{2}$ ($^2\Sigma^+$)	22556.5	[394.73]	Z 1.77 H	0.20762 ^f	0.001430	2.22	2.1597	A \rightarrow X ₂ , R	14226.21	(4)
								A \leftrightarrow X ₁ , R	22502.09	Z (1)(2)* (8)
X ₂ $^2\Pi_{3/2}$	8263.5	[528.75]	Z 1.50 H ^Q	0.23403	0.001450	1.78	2.0342	(X ₂ - X ₁)	8275.88	
X ₁ $^2\Pi_{1/2}$	0	[502.73]	Z 2.28 ^g	0.22875 ^h	0.001473	1.83	2.0575			

PbBr: ^aSee (2) for a discussion of this value.
^bElectron impact study of PbBr₂ (4); the same authors give 0.9 eV for the electron affinity of PbBr.
^c $w_e y_e = -0.028$.
^dTentative rotational analysis (5).
^e(3) give $w_e x_e = 0.52$, $w_e y_e = +0.0023$. Similar constants in (6).
 (1) Morgan, PR 49, 47 (1936).
 (2) Wieland, Newburgh, HPA 25, 87 (1952).
 (3) Pannetier, Deschamps, CR 261, 3109 (1965).
 (4) Hastie, Bloom, Morrison, JCP 47, 1580 (1967).
 (5) Lal, Khanna, CJP 46, 1991 (1968).
 (6) Singh, IJPAP 6, 384 (1968).

PbCl: ^aSee (3) for a discussion of this value.
^bFrom an electron impact study of PbCl₂ by (6) who have also determined the electron affinity of PbCl, E.A. = 1.0 eV.
^cThe revised vibrational analysis of the B←X₁ system by (5a) leads to the expression $v = 34937.5 + 386.3(v' + \frac{1}{2}) - 1.36(v' + \frac{1}{2})^2 - 300.8(v'' + \frac{1}{2}) + 1.04(v'' + \frac{1}{2})^2$ and $v_{00} = 34980.2$.
^dTentative rotational analyses (4)(7).
^e $w_e y_e = -0.07$.
 (1) See ref. (1) of PbBr.
 (2) Rochester, PRS A 153, 407 (1936); 167, 567 (1938).
 (3) See ref. (2) of PbBr.
 (4) Rao, Rao, ZP 181, 58 (1964).
 (5) Pannetier, Deschamps, BSCF (1965), 2933.

PbCl (continued):

(5a) Cordes, Gehrke, ZPC(Frankfurt a. M.) 51, 281 (1966).
 (6) See ref. (4) of PbBr.
 (7) Singh, Singh, CS 37, 282 (1968).
 (8) Singh, IJPAP 8, 114 (1970).

PbF: ^aThermochemical value (mass-spectrom.) (6). See also (3) who consider the possibilities $D_0^0 = 4.54$, 3.57, or 3.22 eV.
^bElectron impact appearance potential (6).
^c(3) consider it possible that the observed C state levels ($v=1\dots 5$) are actually higher vibrational levels of B ²Σ⁺ ($v=5\dots 9$).
^dSpin splitting constant $\gamma = +0.0027$.
^eBreaking off in emission above $v'=1$ (predissociation).
^fΩ-type doubling $\Delta v_{fe}(v=0) = +0.6185(J+\frac{1}{2}) - 10.2 \times 10^{-7}(J+\frac{1}{2})^3$.
^gDetermined from head-origin calculations.
^hΛ-type doubling $\Delta v_{fe}(v=0) = -0.1388(J+\frac{1}{2})$.
 (1) See ref. (1) of PbBr.
 (2) See ref. (2) of PbCl.
 (3) See ref. (2) of PbBr.
 (4) Barrow, Butler, Johns, Powell, PPS 73, 317 (1959).
 (5) Singh, IJPAP 5, 292 (1967).
 (6) Zmbov, Hastie, Margrave, TFS 64, 861 (1968).
 (7) Singh, Singh, Singh, CJP 50, 2206 (1972).
 (8) Lumley, Barrow, JP B 10, 1537 (1977).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(208)Pb ¹ H		$(\mu = 1.00296500) \quad D_0^0 \leq 1.59 \text{ eV}^a$								MAY 1977
C ($^2\Delta$)		Single weak band, not yet analyzed.						C \rightarrow X,	26205	(3)(5)
B ^b	(18030)	[478.8] ^c	Z	[2.478] ^{cd}			[2.604]	B \rightarrow X,	R 17498.7 ^c	(1)(3)
A	(17590)	(500) ^e	(10) ^e	(3.025) ^e	(0.05) ^e		(2.36)	(A-X)	(17060) ^e	
X ($^2\Pi_{1/2}$) ^f	0	1564.1	Z	29.75	4.971	0.144	[201]		1.838 ₈	
(208)Pb ¹²⁷ I		$(\mu = 78.813543_3) \quad D_0^0 = (2.0) \text{ eV}^a$								JUL 1977
B ($^2\Sigma$)	33488.0	198.7	H	0.35	Diffuse bands (prediss.)			B \leftarrow X,	V 33507.1 _b	H (1)*
A ($\frac{3}{2}$)	20529.0	142.0 ^b	H	1.50				A \leftrightarrow X,	R 20519.4 _b	H (1)*
X ($^2\Pi_{1/2}$)	0	160.5	H	0.25						
208Pb ¹⁶⁰		$\mu = 14.8526392_3 \quad D_0^0 = 3.83 \text{ eV}^a$								JUL 1977
Fragments of two further absorption systems in the region 54800 - 57500 cm^{-1} ; not fully published.										(10)
G	51661	540.5	H	6				G \leftarrow X,	R 51570	H (10)
F	51153	558.5	H	3				F \leftarrow X,	R 51072	H (10)
E 0^+	34454	454	H	7	(0.239) ^b	(0.0014)	(2.18)	E \leftrightarrow X,	R 34320	H (2)* (5)
D 1	30198.7	530.5	H	2.92	0.2711 ^{cd}	0.0031	(0.28)	D \leftrightarrow X, ^e	R 30103.5	H (1a)(2)* (5)
										(14)*
C* 1	24947	494	H	3.0	0.248 ^f	0.0018	(0.25)	C* \leftarrow X,	R 24833	H (1a)(5)(10)
C 0^+	23820	532 ^g	H	3.9	0.254	0.002	(0.25)	C \leftarrow X,	R 23725	H (1a)(5)(10)
B 1	22285	498.0 ^h	H	2.20	0.2646 ^{id}	0.0026	(0.30)	B \leftrightarrow X, ^k	R 22173.4	H (1a)(5)(14)*
A 0^+	19862.6	444.3 ^l	H	0.54 ^l	0.2586 ₉ ^d	0.0013 ₈	(0.33)	A \leftrightarrow X, ^e	R 19725.0	H (1)(3)* (5)
										(17)
b 0^-	(16454)	(441)						b \rightarrow X,	R 16315	H (15)(16)
a 1	16024.9	481.5	H	2.4 ₅	(0.25 ₂)		(2.1 ₂)	a \rightarrow X,	R 15905.4	H (15)* (16)
										(17)*
X $1\Sigma^+$	0	721.0	H	3.54 ^m	0.3073056 ^d	0.0019148	(0.22 ₃)	1.921813	Microwave sp. ⁿ	(6)
									Matrix IR sp.	(12a)

PbH: ^aFrom the predissociation in B assuming dissociation at that limit into $^3P_1 + ^2S$.

^b(1)(3) assumed this to be a $^2\Sigma$ state; more recently, (5) suggested that the red system of PbH originates from a $^4\Sigma^-(\frac{1}{2}, \frac{3}{2})$ upper state.

^cStrong perturbations; $\Delta G(3/2 \dots 9/2) = 448.1, 438.5, 432.6, 403; B_1 \dots B_4$ (for low J values) = 2.660, 2.766, 2.770, 2.646. (2) has estimated the following "deperturbed" constants: $\omega_e = 535, \omega_e x_e = 15, B_e = 2.48, \alpha_e = 0.08, T_0 = 17520$.

^dBreaking off (predissociation) at $N'=30, 24, 20$ for $v'=3, 4, 5$, respectively (1). The $v=5, N=20$ level lies at about 20610 cm^{-1} above the lowest ground state level.

^eAll constants estimated from the perturbations in B (2).

^fOriginally believed to be $^2\Sigma$ (1)(3), reassigned by (4)(5). The $^2\Pi_{3/2}$ component is expected at $\sim 8000 \text{ cm}^{-1}$ above $^2\Pi_{1/2}$; the corresponding spectrum is in the infrared and not yet observed.

(1) Watson, PR 54, 1068 (1938).

(2) Gerö, ZP 116, 379 (1940).

(3) Watson, Simon, PR 57, 708 (1940).

(4) Howell, PPS 57, 37 (1945).

(5) Kleman, Thesis (Stockholm, 1953).

PbI: ^aSee the discussion in (1).

^bVibrational numbering uncertain.

(1) Wieland, Newburgh, HPA 25, 87 (1952).

PbO: ^aThermochemical value (mass-spectrom.) (7). From the $\text{Pb} + \text{O}_3$ chemiluminescence spectrum under single-collision conditions (15) derive $D_0^0 \geq 3.74 \text{ eV}$.

^bStrong perturbations make the constants for this state somewhat uncertain. For ^{206}PbO $B_e = 0.2421, \alpha_e = 0.0026$ (10).

PbO (continued):

^cPerturbations in $v=0$ (14).

^dRKR potential functions (8).

^eFranck-Condon factors (4).

^f(10) quotes $B_e = 0.2491$ (extrapol. from $v=6, 7$) for ^{206}PbO .

^gThe vibrational numbering of (1a) has been increased by 2.

^hVibrational constants from (1a); (5) give $\omega_e = 493.5, \omega_e x_e = 2.26$. Irregular vibrational intervals.

ⁱRotational perturbations in $v=1$ (14).

^jLifetimes $\tau[B(v=0, 1)] = 2.58 \text{ } \mu\text{s}, \tau[A(v=2)] = 3.75 \text{ } \mu\text{s}$ (15).

^kRelative intensities (11); transition probabilities (12).

^lConstants derived from band heads with $v' \leq 6$ (17), in good agreement with results quoted by (10) from an unpublished thesis by Travis (rot. anal. of $v=0 \dots 3$ of ^{206}PbO) but considerably smaller than earlier values ($\omega_e = 451.7, \omega_e x_e = 3.33$) proposed by (1).

^mGround state levels observed to $v=15$ (17).

ⁿStark effect (9), $\mu_{el}(v=0) = 4.64 \text{ D}$. Zeeman effect (13), $g_J(v=0) = -0.1623$.

(1) Bloomenthal, PR 35, 34 (1930).

(1a) Howell, PRS A 153, 683 (1936).

(2) Vago, Barrow, PPS 52, 449 (1947).

(3) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(4) Nicholls, Fraser, Jarman, CF 3, 13 (1959).

(5) Barrow, Deutsch, Travis, Nature 191, 374 (1961).

(6) Törring, ZN 19 a, 1426 (1964).

(7) Drowart, Colin, Exsteen, TFS 61, 1376 (1965).

(8) Nair, Singh, Rai, JCP 43, 3570 (1965).

(9) Hoeft, Lovas, Tiemann, Tischer, Törring, ZN 24 a, 1222

(10) Barrow, in DONNSPEC (1970), p.320. (1969).

(11) Dube, Upadhyaya, Rai, JQSRT 10, 1191 (1970).

(continued p. 529)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{31}\text{P}(^{79})\text{Br}$		$(\mu = 22.2436175)$								MAY 1977
b $^1\Sigma^+$	(11782)	[(482.4)] H						b \rightarrow X,	V 11808.6 H	(1)*
X $^3\Sigma^-(0^+)$	0	[(428.4)] H								
$(^{208})\text{Pb}^{32}\text{S}$		$(\mu = 27.7119401) \quad D_0^0 = 3.49 \text{ eV}^a$								JUL 1977
F	47770	370	H (7.8)					F \leftarrow X,	R 47729.5 ^b H	(2)*
E (0^+)	(34000)	Unclassified bands in the region 3100 - 2750 \AA ($32200 - 36400 \text{ cm}^{-1}$).						E \leftarrow X,		(2)*
D 1	29653.2	297.8 ₃	Z 1.36 ₅	0.1016 ₀ ^c	0.00064		2.447	D \leftarrow X, ^d	R 29587.4 Z	(1)(3)
C' (1)	25024.4	283.95	H 1.171					C' \leftarrow X,	R 24952.3 H	(1)
C (0^+)	23212.9	303.93	H 1.436					C \leftarrow X,	R 23150.7 H	(1)
B 1	21847.4	282.1 ₇	H 0.85 ₆	0.0999 ₂ ^c	0.00060 ₂		2.467	B \leftarrow X, ^d	R 21774.5 H	(1)* (3)
A 0^+	18853.0	260.8 ₃	Z 0.36 ₃	0.0963 ₄ ^c	0.00026 ₂		2.513	A \leftarrow X, ^d	R 18768.9 Z	(1)* (3)
a 1	14892.9	285.9	H (0.88)	0.0926 ₇	0.00037 ₄		2.562	a \leftarrow X, ^d	R 14821.9 Z	(3)
X $^1\Sigma^+$	0	429.40	Z 1.30	0.11631868 ^{ec}	0.00043509 ^f	3.415 ^g	2.286863	Vibration sp. ^h		(7a)
								Rotation sp. ⁱ		(5)(9)
$(^{208})\text{Pb}(^{80})\text{Se}$		$(\mu = 57.732425_8) \quad D_0^0 = 3.08 \text{ eV}^a$								JUL 1977
F	45220.9	224.8	H 0.50					F \leftarrow X,	R 45194.5 H	(3)(4)*
D	28418.0	190.4	H 0.53 ^b					D \leftrightarrow X,	R 28374.4 H	(2)* (4)
C	23315.7	183.0	H 0.25					C \leftarrow X,	R 23268.5 H	(1)
B	21005.8	184.8	H 0.43					B \leftarrow X,	R 20959.4 H	(1)
A	18716.8	166.9	H 0.14					A \leftarrow X, ^c	R 18661.5 H	(1)
X $^1\Sigma^+$	0	277.6 ^d	H 0.51 ^d	0.05059953 ^e	0.00012993 ^f	0.70	2.402233	Vibration sp. ^g		(7a)
								Rotation sp. ^h		(5)

PbO (continued):

- (12) Dube, CS 40, 32 (1971).
- (12a) Ogden, Ricks, JCP 56, 1658 (1972).
- (13) Honerjäger, Tischer, ZN 28 a, 1372 (1973).
- (14) Ram, Singh, Upadhyaya, SpL 6, 515 (1973).
- (15) Oldenborg, Dickson, Zare, JMS 58, 283 (1975).
- (16) Kurylo, Braun, Abramovitz, Krauss, JRNBS A 80, 167
- (17) Linton, Broida, JMS 62, 396 (1976). (1976).

PBr: (1) de Bie - Prévot, Thèse (U. Libre de Bruxelles, 1974).

PbS: ^aThermochemical value (mass-spectrom.) (2a), revised (6).

There appears to be a convergence of the E←X bands near 2715 Å (2). If it is assumed that this limit corresponds to ³P₁ + ³P₁ (3) one finds D₀⁰ = 3.54 eV.

^bObserved value. T_e, w_e, w_ex_e represent only v'=1,2,...; the v'=0 bands are displaced by ~12 cm⁻¹ to lower energies owing to a perturbation.

^cRKR potential functions (4).

^dAlso observed as laser-excited emission in Ne, Ar, Kr, SF₆ matrices (8). Lifetimes in solid Ar have been measured for a (260 μs), A (0.95 μs), B (1.8 μs) (8).

^eRotational constants for ²⁰⁸Pb³²S; B_e values for other isotopes and adiabatic corrections (9).

$$f - 5.3_1 \times 10^{-7} (v + \frac{1}{2})^2 - 5.0 \times 10^{-9} (v + \frac{1}{2})^3.$$

$$g \beta_e = + 0.013 \times 10^{-8}.$$

^hIn Ar matrix at 12 K. (8) have also observed the Raman spectrum of the PbS fundamental in solid argon.

ⁱDipole moment of ²⁰⁸Pb³²S, μ_{el}(v=0) = 3.5₉ D, from Stark effect of rotation spectrum (5). A somewhat different value, 4.0₂ D, is given by (7). g_J = -0.06422 [Honerjäger and Tischer, quoted in (9)].

(1) Rochester, Howell, PRS A 148, 157 (1935).

PbS (continued):

- (2) Vago, Barrow, PPS 59, 449 (1947).
- (2a) Colin, Drowart, JCP 37, 1120 (1962).
- (3) Barrow, Fry, Le Bargy, PPS 81, 697 (1963).
- (4) Nair, Singh, Rai, JCP 43, 3570 (1965).
- (5) Hoeft, Lovas, Tiemann, Tischer, Törring, ZN 24 a, 1222
- (6) Uy, Drowart, TFS 65, 3221 (1969). | (1969).
- (7) Murty, Curl, JMS 30, 102 (1969).
- (7a) Marino, Guerin, Nixon, JMS 51, 160 (1974). | (1977).
- (8) Teichman, Nixon, JMS 54, 78; 57, 14 (1975); 65, 258
- (9) Tiemann, Stieda, Törring, Hoeft, ZN 30 a, 1606 (1975).

PbSe: ^aThermochemical value (6) [based on D₀⁰(Se₂) = 3.41 eV].

This value agrees well with D₀⁰ = 3.10 eV derived from a dissociation limit at 2870 Å (4) if dissoc. into ³P₁ + ³P₁ ^bw_ey_e = -0.004. | is assumed.

^cAlso observed as laser-excited emission in Ne matrices

^dAverage of (1) and (2). | (8).

^eRotational constants of ²⁰⁸Pb⁸⁰Se; data for fourteen other isotopic species (5).

$$f \gamma_e = - 1.11 \times 10^{-7}.$$

^gIn Ar matrix at 12 K.

^hDipole moment of ²⁰⁸Pb⁸⁰Se, μ_{el}(v=0) = 3.2₈ D, from Stark effect measurements on microwave transitions (7).

(1) Walker, Straley, Smith, PR 53, 140 (1938).

(2) Barrow, Vago, PPS 56, 76 (1944).

(3) Sharma, Nature 157, 663 (1946).

(4) See ref. (2) of PbS.

(5) Hoeft, Manns, ZN 21 a, 1884 (1966).

(6) See ref. (6) of PbS.

(7) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 539 (1970).

(7a) See ref. (7a) of PbS.

(8) Teichman, Nixon, JMS 57, 14 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-9}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(208)Pb(130)Te										
		$(\mu = 79.961030_2)$		$D_0^0 = 2.5_5 \text{ eV}^a$						JUL 1977
G	46541.7 ^b	159.6	H 1.4					G \leftarrow X, R	46515.3 H	(3)*
F	41658.8	176.4 ^c	H 1.0					F \leftarrow X, R	41640.9 H	(3)*
D	27176.5	142.6	H 1.58					D \leftarrow X, R	27141.5 H	(3)*
B	19737.8	144.9	H 0.45					B \leftrightarrow X, R	19704.3 H	(1)(5)*
A	18405.5	127.0 ₈	H 0.10 ₅					A \leftrightarrow X, ^d R	18363.1 H	(5)*
a	14925.5	146.6 ₄	H 0.24					a \leftarrow X, R	14892.9 H	(7)
X $1\Sigma^+$	0	211.9 ₆	H 0.43	0.03130774 ^e	0.00006743 ₃ ^f	2.7	2.59497 ₅	Microwave sp. ^g		(8)
31P(35)Cl										
		$(\mu = 16.4251442)$		Diffuse bands ^a						JUL 1977 A
B	41234	786	H 27					B \leftarrow X, V	41333 H	(1)
b $1\Sigma^+$	12087	607	H (3.5)					b \rightarrow X, V	12102.1 H	(2)
X $3\Sigma^-(0^+)$	0	577	H 3.5							
(106,108)Pd₂										
		$(\mu = 53.447166)$		$D_0^0 = 0.7_3 \text{ eV}^a$						APR 1975
(106)Pd²⁷Al										
		$(\mu = 21.5030940)$		$D_0^0 = 2.6_0 \text{ eV}^a$						MAY 1976
(106)Pd(11)B										
		$(\mu = 9.9725941)$		$D_0^0 = 3.3_7 \text{ eV}^a$						APR 1975
(106)Pd(74)Ge										
		$(\mu = 43.534131_2)$		$D_0^0 = 2.7_0 \text{ eV}^a$						APR 1975
(106)Pd¹H										
		$(\mu = 0.99832471)$		Complex absorption spectrum 21300 - 24400 cm^{-1} ; strong perturbations.						APR 1975
(A)		Strong band.						(A) \leftarrow X, (R)	22167 H	(1) (4)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(106) Pd ¹ H (continued)										
X 2 Σ^+	0							ESR sp. ^a		(3)

PbTe: ^aThermochemical values of (4) and (6), corrected by (9) for change in value of $D_0^0(\text{Te}_2)$.

^b(2) gives $T_e = 45918.0$.

^cSlightly different constants in (2).

^dA different band system in the same region ($T_e = 16362.3$, $w'_e = 141.4$, $w'_e x'_e = 0.22_4$) was reported earlier by (1) in absorption but not found by (5).

^eRotational constants for $^{208}\text{Pb}^{130}\text{Te}$.

^f $-0.56 \times 10^{-7}(v+\frac{1}{2})^2 - 0.3_7 \times 10^{-9}(v+\frac{1}{2})^3$.

^gDipole moment $\mu_{el}(v=0) = 2.7_3 \text{ D}$ from Stark effect measurements on pure rotational transitions of $^{208}\text{Pb}^{130}\text{Te}$ (10). Zeeman effect (11), $g_J(v=0) = -0.0180_0 \mu_N$ for $^{208}\text{Pb}^{130}\text{Te}$.

(1) Walker, Straley, Smith, PR 53, 140 (1938).

(2) Sharma, Nature 157, 663 (1946).

(3) Vago, Barrow, PPS 59, 449 (1947).

(4) Pashinkin, Novoselova, RJIC 4, 1229 (1959).

(5) Grove, Ginsburg, SA 16, 730 (1960).

(6) Porter, JCP 34, 583 (1961).

(7) Le Bargo, Barrow, PPS 82, 332 (1963).

(8) Tiemann, Hoeft, Schenk, ZN 24 a, 787 (1969).

(9) Uy, Drowart, TFS 65, 3221 (1969).

(10) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 539 (1970).

(11) Honerjäger, Tischer, ZN 29 a, 1695 (1974).

PCl: ^aObserved in the flash photolysis of PCl_3 .

(1) Basco, Yee, CC (1967), 1146.

(2) de Bie-Prévot, Thèse (U. Libre de Bruxelles, 1974).

Pd_2 : ^aThermochemical value (mass-spectrom.) (1)(2).

(1) Ackerman, Stafford, Verhaegen, JCP 36, 1560 (1962).

(2) Lin, Strauss, Kant, JCP 51, 2282 (1969).

PdAl : ^aThermochemical value (mass-spectrom.) (1).

(1) Cocke, Gingerich, Chang, JCS FT I 72, 268 (1976).

PdB : ^aThermochemical value (mass-spectrom.) (1).

(1) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart, TFS 66, 809 (1970).

PdGe : ^aThermochemical value (mass-spectrom.) (1).

(1) Peeters, Vander Auwera-Mahieu, Drowart, ZN 26 a, 327 (1971).

Pd^1H : ^aIn rare gas matrices at 4 K.

(1) }

(3) } See the corresponding ref. of Pd^2H (p. 533).

(4) }

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{108}\text{Pd}^2\text{H}$										
		$\mu = 1.97719645$								APR 1975
(E) ($^2\Sigma$)				$[2.94]^a$				(E) \leftarrow X, R	24670.48 Z	(1)(2)*
(D) ($^2\Sigma$)				$[2.12]^a$				(D) \leftarrow X, R	23866.87 Z	(2)
(C) ($^2\Sigma$)				$[2.57]^a$				(C) \leftarrow X, R	23483.42 Z	(2)
(B) ($^2\Sigma$)				$[1.99]^a$				(B) \leftarrow X, R	23073.43 Z	(2)
(A) ($^2\Sigma$)				$[3.09]^a$				(A) \leftarrow X, R	22264.06 Z	(2)
X $^2\Sigma^+$	0	1446.02	Z 19.59	3.6489 ^b	0.0812	93.0 ^c	1.5285 ₉	ESR sp. ^d		(3)
$(^{106})\text{Pd}^{16}\text{O}$										
		$(\mu = 13.8961401_2) \quad D_0^0 = 2.8_7 \text{ eV}^a$								APR 1975
$(^{106})\text{Pd}(^{28})\text{Si}$										
		$(\mu = 22.1306028) \quad D_0^0 = 3.2_1 \text{ eV}^a$								APR 1975
$^{31}\text{P}^{19}\text{F}$										
		$\mu = 11.7755965$								JUL 1977
		R shaded triple heads in the region $15600 - 17900 \text{ cm}^{-1}$, tentatively assigned by (4) to a triplet system of PF with $w'' \approx 1135$, probably belong to the D \rightarrow B system of PO (0-0, 0-1, 0-2 bands). Several unassigned bands in the region $16200 - 25500 \text{ cm}^{-1}$ (4).								
g $^1\Pi$	[52063.6]			[0.6186]		[0.85]	[1.521 ₃]	g \rightarrow b, V	38277.74 Z	(1)
d $^1\Pi$	36024	[413.19]	Z a	0.4848	(0.0062)	[2.8]	1.718	g \rightarrow a, V	44544.80 Z	(1)
								d \rightarrow b, R	22444.95 Z	(1)*
								d \rightarrow a, R	28712.14 Z	(1)
B $\begin{cases} 3\Pi_2 \\ 3\Pi_1 \\ 3\Pi_0 \end{cases}$	$\begin{matrix} 29827 \\ 29686 \\ 29543 \end{matrix}^b$	$\begin{matrix} [435.86] \\ [435.91] \\ [436.06] \end{matrix}$	$\begin{matrix} Z \\ Z \\ Z \end{matrix}$	$\begin{matrix} 0.4693 \\ 0.4663 \\ 0.4632^d \end{matrix}$	$\left. \begin{matrix} \\ \\ \end{matrix} \right\} 0.0038^e$		1.752 ₂	B \rightarrow X, R	$\begin{cases} 29623.06 \\ 29481.80 \\ 29338.68 \end{cases} Z$	(1)*
b $^1\Sigma^+$	13353.90	866.14	Z 4.51	0.5725	0.0045	[0.9]	1.581 ₃	b \rightarrow X, V	13363.59 Z	(3)*
a $^1\Delta$	7090.43	858.79	Z 4.438 ^f	0.5699	0.00467	[1.0]	1.584 ₉			
X $^3\Sigma^-$	0	846.75	Z 4.489 ^g	0.5665 ^h	0.00456		1.589 ₇			

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
31P19F+										JUL 1977
A $^2\Sigma$	35434.64	619.00	Z 4.62	0.5593 ⁱ	0.0079	1.6	1.599 ₉	A→X, R	35217.62 Z	(1)
X $^2\Pi_r$	0 ^j	1053.25	Z 5.05	0.6360	0.0048	0.6	1.500 ₃			

Pd²H: ^aEffective B values at N=0. All levels strongly perturbed. Neither the vibrational numbering nor the number of electronic states involved is known.
^bSpin splitting constant $\gamma_v = -2.262 - 0.051(v + \frac{1}{2})$; slight N dependence.
^c $\beta_e = -1.0 \times 10^{-6}$.
^dIn rare gas matrices at 4 K.
(1) Lagerqvist, Neuhaus, Scullman, PPS 83, 498 (1964).
(2) Malmberg, Scullman, Nylén, AF 39, 495 (1969).
(3) Knight, Weltner, JMS 40, 317 (1971).
(4) Scullman, Dissertation (Stockholm, 1971); see USIP Report 71-02.

PdO: ^aThermochemical value (mass-spectrom.) (1).
(1) Norman, Staley, Bell, JPC 68, 662 (1964); 69, 1373 (1965).

PdSi: ^aThermochemical value (mass-spectrom.) (1).
(1) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart, TFS 66, 809 (1970).

PF, PF⁺:

^a $\Delta G(3/2 \dots 7/2) = 416.57, 418.96, 420.98$.
^b $A_0 = +143.06$, $A_1 = +142.87$; see (2) who also accounts for spin-rotation interaction and for the combined effects of spin-spin interaction and perturbations by $^1\Pi$ states.
^c $\Delta G(3/2) = 437.37$.
^d Λ -type doubling independent of J, $\sim 0.07, 0.16, 0.25 \text{ cm}^{-1}$ for $v=0,1,2$, respectively (1).
^eNotice that Table VIII of (1) contains a number of misprints leading to disagreement with constants in Table XI.
^f $w_e y_e = +0.0147$.
^g $w_e y_e = +0.019$.
^hSpin splitting constants $\lambda_0 = +2.9623$, $\gamma_0 = +0.0018$.
ⁱSpin splitting constant $\gamma = 0.0073$.
^j $A = +323.95$.
(1) Douglas, Frackowiak, CJP 40, 832 (1962).
(2) Kovács, CJP 42, 2180 (1964).
(3) Colin, Devillers, Prévot, JMS 44, 230 (1972).
(4) Skolnik, Goodfriend, JMS 50, 202 (1974).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$3\text{IP}^1\text{H}$										
d 1Π B $3\Pi_0$ c 1ϕ A $3\Pi_i$ b $1\Sigma^+$ a 1Δ X $3\Sigma^-$	 0 ⁺ 29498 ^d 0 ⁻ 1 2 (15160) ^k (7660) ^k 0	 [1833.78] Z [1833.39] Z [1833.74] Z [1834.38] Z (98.5) ^e 2365.2 ^m 44.5 ^m	 [8.478] ^b [7.3] [8.60] ₂ [8.0222] ^f 8.5371 ⁿ	 0.21 g 0.12 0.2514	 [4.17] [5.44] [5.683] ^h [4.18] 4.36	 [1.427] ₃ [1.54] [1.417] ₀ [1.46728] [1.4302] 1.4223 ₄	d← a, B← X, R c← a, ^c A ⁱ ↔ X, R Rotation sp. ^l Rotation sp. ^l	62725.28 Z 69587.8 Z 61548.68 Z $\left\{ \begin{array}{l} 29434.61^j \\ 29434.28^j \\ 29316.81^j \\ 29203.21^j \end{array} \right.$ 		

P^1H , P^2H :

^aAdjusted theoretical value recommended by (15); see also (6)(8)(12).

^b Λ -type doubling $|\Delta v| = 0.1275 J(J+1) - 0.54 \times 10^{-4} J^2(J+1)^2$.

^cSequence of nearly undegraded bands; the origins of the 1-1 and 2-2 bands are at 61554.5 and 61560.7 cm^{-1} , resp..

^d $A_0 = -115.71$, $A_1 = -115.20$; see (13) who give also centrifugal distortion corrections A_D as well as estimated spin-spin and second-order spin-orbit parameters.

^eEstimated using isotope relations.

^fFor Λ -doubling constants see (13).

^g $B_1 = 7.549_2$. No emission has been observed from $v=1$ of P^1H , probably owing to weak predissociation by the repulsive $^5\Sigma^-$ state arising from ground state atoms (13).

^h $D_1 = 6.54 \times 10^{-4}$, $H_0 = -1.6 \times 10^{-8}$.

ⁱLifetime 0.45 μs , corresponding to an absorption oscillator strength of 0.0078 (7).

^jSubband origins as defined by (13).

^kTheoretical predictions (6)(10)(12), for $a^1\Lambda$ confirmed by laser photoelectron spectrometry of PH^- [see ref.(3) of PH^-].

^l $N=4 \rightarrow 5$ rotational transitions observed by the laser magnetic resonance method.

^mConstants deduced from isotope relations (13).

ⁿSpin splitting constants $\lambda_0 = +2.21_2$, $\gamma_0 = -0.073_8$;

$\lambda_1 = +2.20_7$, $\gamma_1 = -0.072_6$ (13).

^oFrom the value for P^1H .

^p $A_0 = -115.74$, $A_1 = -115.55$; see also ^d.

^q $B_1 = 4.004_7$.

^r $D_1 = 1.640 \times 10^{-4}$.

^sSpin splitting constants $\lambda_0 = +2.21_1$, $\gamma_0 = -0.038_5$;

$\lambda_1 = +2.20_2$, $\gamma_1 = -0.038_1$ (13).

(1) Pearse, PRS A 129, 328 (1930).

P^1H , P^2H (continued):

(2) Ishaque, Pearse, PRS A 156, 221 (1936).

(3) Ishaque, Pearse, PRS A 173, 265 (1939).

(4) Legay, CJP 38, 797 (1960).

(5) Kovács, APH 13, 303 (1961).

(6) Jordan, JCP 41, 1442 (1964).

(7) Fink, Welge, ZN 19 a, 1193 (1964).

(8) Cade, Huo, JCP 47, 649 (1967).

(9) Horani, Rostas, Lefebvre-Brion, CJP 45, 3319 (1967).

(10) Cade, CJP 46, 1989 (1968).

(11) Balfour, Douglas, CJP 46, 2277 (1968).

(12) Liu, Legentil, Verhaegen, in "Selected Topics in Molecular Physics" (ed. Clementi), p.19. Chemie GmbH (1972).

(13) Rostas, Cossart, Bastien, CJP 52, 1274 (1974).

(14) Davies, Russell, Thrush, CPL 36, 280 (1975).

(15) Meyer, Rosmus, JCP 63, 2356 (1975).

P^1H^+ , P^2H^+ :

^aFrom the predissociation in $A^2\Delta(v=0)$. A rough extrapolation of the A state to the dissociation limit $^1D + ^2S$ leads to $D_0^0 \approx 3.0_6$ eV (1).

^b $A_0 = +1.38$, $A_1 = +0.82$.

^cSpin-rotation interaction constant $\gamma = 0.175$. There is a sudden breaking off in $v=0$ above $N=12$.

^d $B_1 = 6.558_8$. All lines originating from F_1 levels of $v=1$ are much weaker than those arising from F_2 .

^eRefers to the zero-point of the Hill-Van Vleck expression for both upper and lower state.

^f $A_0 = +295.9_4$, $A_1 = +296.2$.

^g Λ -type doubling constants for $v=0$: $|p| = 0.23$, $|q| = 0.011$.

(continued p. 537)

P^1H^+ , P^2H^+ (continued):

$$^hB_1 = 8.145_0.$$

$$^iA_0 = + 1.35.$$

$$^j\text{Spin-rotation interaction constant } \gamma = 0.096.$$

$$^kA_0 = + 295.83.$$

$$^l\Lambda\text{-type doubling constant } |p| = 0.08.$$

(1) Narasimham, CJP 35, 901 (1957).

(2) Narasimham, Dixit, CS 36, 1 (1967).

P^1H^- : ^aFrom $D_0^0(P^1H)$ and the electron affinities of PH and H. Notice, however, that the ground $^2\Pi$ state of PH^- cannot dissociate into $P(^4S) + H(^1S)$ but must correlate with the slightly higher limit $P(^3P) + H(^2S)$ at 3.31 eV. The atomic electron affinities are taken from (2).

^bFrom the photodetachment spectrum (3).

^c $A = -212 \text{ cm}^{-1}$ [theoretical value (1)].

^dFranck-Condon factor analysis of the photodetachment spectrum (3).

(1) Walker, Richards, JCP 52, 1311 (1970).

(2) Hotop, Lineberger, JPCRD 4(3), 539 (1975).

(3) Zittel, Lineberger, JCP 65, 1236 (1976).

PI: (1) de Bie-Prévoit, Thèse (U. Libre de Bruxelles, 1974).

PN, PN^+ :

^aLatest thermochemical value (mass-spectrom.) (6). Previous thermochemical value 7.57 eV (5). The origin of the discrepancy is not clear. From ab initio calculations a value of 6.43 eV is obtained; see (6).

^bFrom the photoelectron spectrum (12).

^cPotential functions (3).

^dLifetime $\tau(v=0) = 0.23 \text{ } \mu\text{s}$ [Hanle effect measurement (11)].

^eRelative transition probabilities from the fluorescence spectrum, Franck-Condon factors (10); see also (4).

$$f - 6.4_0 \times 10^{-6}(v+\frac{1}{2})^2 - 2.5 \times 10^{-7}(v+\frac{1}{2})^3 \text{ (9).}$$

$$^g\mu_{el}[D] = 2.7514 - 0.0086(v+\frac{1}{2}), \text{ as corrected by (9) for improved } B_v \text{ values; (eqQ)}_N[\text{kHz}] = -5172.8 + 60.7(v+\frac{1}{2}). \text{ (7)}$$

give also magnetic hf coupling constants.

^hFrom $D_0^0(PN)$, I.P.(PN), and I.P.(P).

(1) Curry, Herzberg, Herzberg, ZP 86, 348 (1933).

(2) Moureu, Rosen, Wettruff, CR 209, 207 (1939).

(3) Singh, Rai, IJPAP 4, 102 (1966).

(4) Smith, JP B 1, 89 (1968).

(5) Uy, Kohl, Carlson, JPC 72, 1611 (1968).

(6) Gingerich, JPC 73, 2734 (1969).

(7) Raymonda, Klemperer, JCP 55, 232 (1971).

(8) Hoeft, Tiemann, Törring, ZN 27 a, 703 (1972).

(9) Wyse, Manson, Gordy, JCP 57, 1106 (1972).

(10) Moeller, Silvers, CPL 19, 78 (1973).

(11) Moeller, McKeever, Silvers, CPL 31, 398 (1975).

(12) Wu, Fehlner, CPL 36, 114 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{31}\text{P}^{16}\text{O}$		$\mu = 10.5479381_1$ $D_0^0 = 6.15 \text{ eV}^a$ I.P. = $(8.2_3) \text{ eV}^b$								SEP 1977
		Theoretical calculations of the ground state (11)(21), of low-lying valence states (29)(30), and of Rydberg states (22).								
H $^2\Sigma^+$	(56017) ^c	(1391)	(7)	(0.780)	(0.005 ₄)		(1.431)	H→B, R_V (25401) ^d		(20a)* (33)*
I $^2\Sigma^+$	55458.1	1390.2	Z 6.0	0.7798 ^e	0.0048	0.8	1.4316	I→A, 15051.1 Z		(24)*
								I→B, V 24842.0		(20a)* (33)*
								I→X, V 55536.7		(33)*
E $^2\Delta$	53091	[1456.28]	Z (15.8)	0.758 ₃ ^f	0.0074	0.8	1.451 ₈	E→X, V 53215.6 Z		(1)* (25)* (35)*
G $^2\Sigma^+$	(52412) ^c	(1382)	(13)	(0.780)	(0.005 ₄)		(1.431)	G→A, (11999) ^d		(31)*
								G→B, R_V (21790) ^d		(20a)* (33)*
								G→X, V (52484) ^d		(33)*
F $^2\Sigma^+$	(49880) ^c	(850)	(7.5)	(0.608 ₂)	(0.0045)		(1.621)	F→A, R (9202) ^d		(33)*
								F→B, R (18993) ^d		(20a)* (24) (33)*
								F→X R (49688) ^d		(33)*
D $^2\Pi_r$	48520 ^g	[1358.1]	(7)	0.755 ^h	0.007		1.455	D→B, R 17894.6 ^d		(15)(18)* (34)*
								D↔X, R 48589.3 ^d		(1)(15)(18)* (40)*
C $^2\Sigma^-$	44831.7 ₅	779.2 ₂ ⁱ	Z 5.14	0.590 ₃ ⁱ	0.0056	(1.4)	1.645	C→X, R 44605.0 ₅ Z		(1)(20)(23)* (32)*
C' $^2\Delta$	43742.7 ₄	825.7 ₄	Z 6.93 ^j	0.640 ₅ ^k	0.0052	(1.5)	1.580	C'→X, R 43538.8 ₅ Z		(5)(6)(8)* (16)(20) (23)* (32)*
A $^2\Sigma^+$	40406.8 ₉	1390.9 ₄ ^l	Z 6.91 ^l	0.7801 ^{lmn}	0.0054 ₂ ^l	1.0	1.4313	A→B, V_R 9790.86 Z		(20a)* (24)* (31)*
								A↔X, ^o V 40485.60 Z		(2)* (4)(12) (16)* (36)*
								γ bands		

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$31\text{P}^{16}\text{O}$ (continued)										
$B', ^2\Pi$	33120.7 ^p	759.2 ^q	3.8 ₅ ^q	0.5420 ^q	0.0049 ^q	[1.0]	1.717 ₂	$B' \rightarrow B, ^r R$ $B' \leftrightarrow X, R$	32884.3 ^q	(34)* (19)(20)(37) (40)*

PO: ^aThermochemical value (mass-spectrom.) (27). The predissociation in the perturbed $D(v=0)$ level (see ^h) gives the upper limit $D_0^0 \leq 6.161$ eV.

^bTheoretical value (22). (27) report an electron impact appearance potential of 8.5 eV.

^cThe G, H, I $^2\Sigma^+$ Rydberg states (as well as higher levels of A $^2\Sigma^+$) interact with the F $^2\Sigma^+$ non-Rydberg state. Most of the observed bands are strongly perturbed. The constants in the Table are deperturbed values taken from (33) who give results for P^{16}O and P^{18}O ; similar constants have earlier been reported by (20a). In addition to the strong homogeneous interactions a large number of local perturbations have been described for both isotopes (20a)(24)(33).

^dThe v_{00} values have been calculated from deperturbed constants and should not be expected to coincide precisely with observed transitions.

^eRotational perturbations in $v=0,1,2$ (24).

^fPerturbations by $C' \ ^2\Delta$.

^g $A_0 = +26.2$, $A_1 = +22.8$. All constants given for $D \ ^2\Pi$ ($v=0,1$) are deperturbed values from (40); see also (34). This state interacts strongly with high vibrational levels of $B' \ ^2\Pi$. For $v=2$ and 3 only fragments have been observed in absorption (40) making the deperturbation results for these levels even less reliable.

^hThe highest level observed in emission from the interacting pair $D(v=0) \sim B'(v=24?)$ is the $N=34$ level [predominantly $D(v=0)$] lying at 49647 cm^{-1} above $X \ ^2\Pi_{1/2}$ ($v=0, J=1/2$); see (15). Higher levels are predissociated and give rise to diffuse lines in the absorption spectrum. A summary of predissociation phenomena observed in B' and D levels is given by (40) who suggest that the predissociation is caused by the repulsive part of the $^4\Pi$ state arising from $^4S + ^3P$.

ⁱVibrational numbering confirmed by $\text{P}^{16}\text{O} - \text{P}^{18}\text{O}$ isotope shifts (32).

^j(35) suggest that an additional term, $w_e v_e \approx +0.040$, is needed in order to account for higher vibrational levels ($v=14 \dots 18$) found in perturbations of $E \ ^2\Delta$ ($v=0,1,2$).

^kSmall spin doubling, $\gamma \approx 0.0085$ (32); local perturbations.

^lAverage of values obtained by (2)(31)(36). Above $v=3$ the influence of the F $^2\Sigma^+$ state becomes noticeable.

^mSpin splitting constant $\gamma = +0.0013$ (31). Many rotational perturbations (26)(31)(36).

ⁿPotential curves (7).

^oFranck-Condon factors (10).

^p A_v increases from -13.3 for $v=0$ to about +30 for $v=23 \dots 26$ (19)(34)(40); theoretical explanation (29).

^qThese are the constants of (31) based on the rotational (continued p. 540)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$31\text{P}^{16}\text{O}$ (continued)										
b $4\Sigma^-$	(34837) ^s	(889.0) ^s	(6.6 ₂) ^s	(0.644) ^s	(0.006) ^s		(1.57 ₅)			
B $2\Sigma^+$	30730.88	1164.51	Z 13.46 ^t	0.7463 ^{un}	0.0088 ^v	1.25	1.4634	B \leftrightarrow X, V_R	30694.74 Z	(1)* (4)(9)* (14)(16)* (28)(37)* ^w
X $2\Pi_r$	0 ^x	1233.34	Z 6.56	0.7337 ^{yn}	0.0055	1.3	1.4759	β bands		
$31\text{P}^{16}\text{O}^+$										
$D_0^0 = (8.4_1) \text{ eV}^a$										JUL 1977
A $1\Sigma^+$	49930	1017	H 8					A \rightarrow X, R	49735 H	(1)
X $1\Sigma^+$	0	1405	H (5)							
$31\text{P}^{16}\text{O}^-$										
$D_0^0 = 5.78 \text{ eV}^a$ I.P. = 1.09 ₂ eV ^b										JUL 1977
SCF calculations (1).										
a 1Δ	4470	[1020] ^b								
X $3\Sigma^-$	0	[1000] ^b					1.54 ₀ ^c			
210Po_2										
$\mu = 104.991442$ $D_0^0 = (1.90) \text{ eV}^a$										JUL 1977
A	25149.3	108.532	H 0.4417					A \rightarrow X, R	25125.7 H	(1)
X	0	155.715	H 0.3353 ^b							

PO (continued):

analysis of $v=0$ and 1 (19) and on the identification of several intermediate levels ($v=6$ and 12...22) in perturbations with B $2\Sigma^+$ (37) and A $2\Sigma^+$ (31). Higher vibrational levels ($v=23$...26, formerly D' 2Π) are observed in the region of strong interaction with the Rydberg D 2Π state (34)(40). The vibrational numbering chosen by (19) and used in this Table is arbitrary and may have to be in-

creased by 2 as suggested by (41) whose re-analysis of the B'-X system includes a large number of absorption bands previously attributed to OPC1 (39) as well as a number of emission bands left unassigned by (20) and (37).

^rThe B' \rightarrow B bands originate from highly excited levels with $v' \approx 24$ which are strongly mixed with low vibrational levels of D 2Π .

PO (continued):

^sConstants derived from perturbations in B $2\Sigma^+$ and A $2\Sigma^+$ (37), corrected for the new vibrational numbering of (36).

^t $w_e y_e = -0.05$.

^uSpin splitting constant $\gamma = -0.0068$. Extensive rotational perturbations in $v=6,7$ by levels of B' 2Π and b $4\Sigma^-$; see (37). The $v=7$ level appears to be preferentially populated in the P_4+0 glow (20).

^v $y_e = -0.00006$.

^wPapers by (3)(13)(17) contain erroneous branch identifications; see (18)(28).

^x $A_v = 224.03 + 0.18v - 0.013v^2$ ($v \leq 11$) (37); see also (38). Similar results in (32).

^y Λ -type doubling $\Delta v_{ef}(^2\Pi_{\frac{1}{2}}) = -0.0070(J+\frac{1}{2})$.

- (1) Dressler, HPA 28, 563 (1955).
- (2) Rao, CJP 36, 1526 (1958).
- (3) Singh, CJP 37, 136 (1959).
- (4) Norrish, Oldershaw, PRS A 262, 10 (1961).
- (5) Santaram, Rao, ZP 168, 553 (1962); IJP 37, 14 (1963).
- (6) Narasimham, Dixit, Sethuraman, PIAS A 62, 314 (1965).
- (7) Singh, Rai, JPC 69, 3461 (1965).
- (8) Guenebaut, Couet, Coquart, JCPPB 63, 969 (1966).
- (9) Meinel, Krauss, ZN 21 a, 1520, 1878 (1966).
- (10) Sankaranarayanan, IJP 40, 678 (1966).
- (11) Boyd, Lipscomb, JCP 46, 910 (1967).
- (12) Coquart, Couet, Ngo, Guenebaut, JCPPB 64, 1197 (1967).
- (13) Mohanty, Upadhyaya, Singh, Singh, JMS 24, 19 (1967).
- (14) Couet, Ngo, Coquart, Guenebaut, JCPPB 65, 217 (1968).
- (15) Couet, Coquart, Ngo, Guenebaut, JCPPB 65, 1241 (1968).
- (16) Dixit, Narasimham, PIAS A 68, 1 (1968).
- (17) Mohanty, Rai, Upadhyaya, PIAS A 68, 165 (1968).
- (18) Verma, Dixit, CJP 46, 2079 (1968).

PO (continued):

- (19) Verma, CJP 48, 2391 (1970).
- (20) Verma, Broida, CJP 48, 2991 (1970).
- (20a) Verma, Dixit, Jois, Nagaraj, Singhal, CJP 49, 3180
- (21) Mulliken, Liu, JACS 93, 6738 (1971). | (1971).
- (22) Ackermann, Lefebvre-Brion, Roche, CJP 50, 692 (1972).
- (23) Coquart, Couet, Guenebaut, Larzillière, Ngo, CJP 50, 1014 (1972).
- (24) Guha, Jois, Verma, CJP 50, 1579 (1972).
- (25) Coquart, Larzillière, Ngo, CJP 50, 2945 (1972).
- (26) Coquart, Prudhomme, CR B 275, 383 (1972).
- (27) Drowart, Myers, Szwarc, Vander Auwera-Mahieu, Uy, JCS FT II 68, 1749 (1972).
- (28) Rai, Rai, Upadhyaya, JP B 5, 1038 (1972).
- (29) Roche, Lefebvre-Brion, JCP 59, 1914 (1973).
- (30) Tseng, Grein, JCP 59, 6563 (1973).
- (31) Verma, Jois, CJP 51, 322 (1973).
- (32) Prudhomme, Larzillière, Couet, CJP 51, 2464 (1973).
- (33) Ngo, Da Paz, Coquart, Couet, CJP 52, 154 (1974).
- (34) Coquart, Da Paz, Prudhomme, CJP 52, 177 (1974).
- (35) Prudhomme, Coquart, CJP 52, 2150 (1974).
- (36) Coquart, Da Paz, Prudhomme, CJP 53, 377 (1975).
- (37) Verma, Singhal, CJP 53, 411 (1975).
- (38) Zaidi, Verma, CJP 53, 420 (1975).
- (39) Verma, Nagaraj, JMS 58, 301 (1975).
- (40) Ghosh, Nagaraj, Verma, CJP 54, 695 (1976).
- (41) Cornet, Dubois, Houbrechts, JP B 10, L415 (1977).

PO^+ }
 PO^- } See p. 543.
 PO_2 }

PrO: ^aThermochemical value (mass-spectrom.)(3)(4), recalculated (5)(6).

^bCorrected electron impact appearance potential (10).

^cRotational constants obtained by (8):

System X: $B_0' = 0.3459$, $D_0' = 3.1 \times 10^{-7}$, $r_0' = 1.842$;

$B_0'' = 0.3620$, $D_0'' = 2.4 \times 10^{-7}$, $r_0'' = 1.801$.

System VII: $B_1' = 0.3418$, $D_1' = 2.4 \times 10^{-7}$;

$B_0' = 0.3414$, $D_0' = 1.1 \times 10^{-7}$, $r_0' = 1.854$;

$B_1'' = 0.3595$, $D_1'' = 2.6 \times 10^{-7}$;

$B_0'' = 0.3610$, $D_0'' = 2.6 \times 10^{-7}$, $r_0'' = 1.803$;

(B, D in cm^{-1} , r in Å). The upper state of system VII is perturbed. Different rotational constants and band origins have been obtained by (7).

^d(7) suggest that systems VII and IX form the two components of a doublet system.

(1) Watson, PR 53, 639 (1938).

(2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(3) Walsh, Dever, White, JPC 65, 1410 (1961).

(4) Ames, Walsh, White, JPC 71, 2707 (1967).

(5) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

(6) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

(7) Venkitachalam, Krishnamurty, Narasimham, PIAS A 76, 113 (1972).

(8) Shenyavskaya, Egorova, Lupanov, JMS 47, 355 (1973).

(9) Gabelnick, Reedy, Chasanov, JCP 60, 1167 (1974).

(10) Ackermann, Rauh, Thorn, JCP 65, 1027 (1976).

PO⁺: ^a $D_0^0(\text{PO}) + \text{I.P.}(\text{P}) - \text{I.P.}(\text{PO})$.

(1) Dressler, HPA 28, 563 (1955).

PO⁻: ^aFrom $D_0^0(\text{PO})$ and the electron affinities of PO and O.

^bFrom the laser photoelectron spectrum of PO⁻ (2).

^cFranck-Condon factor analysis of the PO⁻ photodetachment peaks (2).

(1) Boyd, Lipscomb, JCP 46, 910 (1967).

(2) Zittel, Lineberger, JCP 65, 1236 (1976).

PO₂: ^aExtrapolation of the lower state vibrational levels.

^b $w_e y_e = -0.0003226$.

(1) Charles, Timma, Hunt, Pish, JOSA 47, 291 (1957).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References		
								Design.	v_{00}			
$^{141}\text{Pr}(^{32})\text{S}$		$(\mu = 26.0592154) \quad D_0^0 = 5.2_1 \text{ eV}^a$								APR 1975		
$^{31}\text{P}^{32}\text{S}$		$\mu = 15.7325008 \quad D_0^0 = 4.5_4 \text{ eV}^a$								JUL 1977		
C	$^2\Sigma$ 34686.5	534.8	H ^Q	3.31	0.00196	2.5	2.013 ₀	C→X, R	34263.5 34584.3	H ^Q	(1)(2)(3)* (4)*	
B	$^2\Pi$ 22987.7 22894.0	512.2	H	2.15				B→X, R	22553.7 22780.8	H	(2)(3)*	
X	$^2\Pi_r$ 320.8 ^c 0	739.1	H ^Q	2.96				[0.2967 ₄] [0.2963 ₂]	[2.0]	[1.900 ₉]		
$^{31}\text{P}^{32}\text{S}^+$										JUL 1977		
A	$(^1\Sigma)$ 40617.5	607.5	H	4.5				A→X, R	40498.7	H	(1)(2)	
X	$^1\Sigma^+$ 0	844.6	H	3.3								
$^{31}\text{P}(^{80})\text{Se}$		$(\mu = 22.3222031) \quad D_0^0 = 3.7_3 \text{ eV}^a$								JUL 1977		
$(^{194},^{195})\text{Pt}_2$		$(\mu = 97.231234)$								AUG 1976		
A		218.4 ^a	0.9					A←X, ^a	11248.7		(1)	
X	0											
$(^{195})\text{Pt}(^{111})\text{B}$		$(\mu = 10.4208585) \quad D_0^0 = 4.9_1 \text{ eV}^a$								MAY 1975		
$^{195}\text{Pt}^{12}\text{C}$		$\mu = 11.30422952 \quad D_0^0 = 6.28 \text{ eV}^a$								MAY 1975		
B	$^1\Sigma^{(+)}$ (32779)	[843.8]	H	bc	0.468 ^c	0.006	7	1.78 ₅	B←X, R	32676.8	H	(3)* (5)(6)*
A	$^1\Pi$ 18627.01	818.74	Z	5.44	0.48023 ^d	0.00411	6.7	1.7621 ₉	A←X, R	18510.67	Z	(1)(3)* (6)
A'	$^1\Pi$ 13262.8	[906.93]	Z	5.6 H	0.50584 ^e	0.00390	6.20 ^f	1.7170 ₀	A'←X, R	13196.14	Z	(2)(5)(6)
A''	$^1\Sigma^{(+)}$ 12697.16	943.40	Z	5.28	0.50957	0.00370 ₅	6.04 ^g	1.7107 ₁	A''←X, R	12643.19	Z	(5)(6)*
X	$^1\Sigma^{(+)}$ 0	1051.13	Z	4.86	0.53044	0.003273	5.46 ^h	1.6767 ₂				

State	T_e	w_e	$w_e x_e$	B_e	e	D_e (10^{-1} cm $^{-1}$)	r_e (Å)	Observed Transitions Design. v_{00}	References
$31p(130)Te$		$(\mu = 25.0104736) \quad D_0^0 = 3.05 \text{ eV}^a$							JUL 1977

PrS: ^aThermochemical value (1), recalculated (2).

(1) Cater, Holler, Fries, quoted in ref. (5) of PrO.

(2) See ref. (6) of PrO.

PS, PS⁺:

^aThermochemical value (mass-spectrom.) (5).

^bSpin doubling constant $\gamma = 0.015_2$.

^c $A_0 = +321.9_3$, from the rotational analysis of the C \rightarrow X 1-0 and 2-0 bands (4).

(1) Dressler, Miescher, PPS A 68, 542 (1955).

(2) Dressler, HPA 28, 563 (1955).

(3) Narasimham, Subramanian, JMS 22, 294 (1969).

(4) Narasimham, Balasubramanian, JMS 37, 371 (1971).

(5) Drowart, Myers, Szwarc, Vander Auwera-Mahieu, Uy, HTS 5, 482 (1973).

PSe: ^aThermochemical value (mass-spectrom.)(1), based on $D_0^0(\text{Se}_2) = 3.2_9 \text{ eV}$.

(1) See ref. (5) of PS.

Pt₂: ^aIn Ar matrix at 12 K; not observed in the gas phase.

(1) Jansson, Scullman, JMS 61, 299 (1976).

PtB: ^aThermochemical value (mass-spectrom.)(1).

(1) McIntyre, Vander Auwera-Mahieu, Drowart, TFS 64, 3006 (1968).

PtC: ^aThermochemical value (mass-spectrom.) (4)(7).

^b $\Delta G(3/2) \approx 808.9$.

^c $B^1\Sigma$ is strongly perturbed.

^d Λ -type doubling $\Delta v_{ef}(v=0) = +0.64 \times 10^{-4} J(J+1)$.

^e Λ -type doubling $\Delta v_{ef}(v=0) = +2.18 \times 10^{-4} J(J+1)$.

^f $H_0 = +7.0 \times 10^{-13}$.

^g $\beta_e = +0.06 \times 10^{-7}$; $H_0 = +5.4 \times 10^{-13}$, $H_1 = +6.6 \times 10^{-13}$.

^h $\beta_e = +0.03 \times 10^{-7}$; $H_0 \dots H_2(10^{-13} \text{ cm}^{-1}) = +8.6, +9.9, +8$.

(1) Neuhaus, Scullman, Yttermo, ZN 20 a, 162 (1965).

(2) Appelblad, Barrow, Scullman, PPS 91, 260 (1967).

(3) Scullman, Yttermo, AF 33, 231 (1967).

(4) Vander Auwera-Mahieu, Drowart, CPL 1, 311 (1967).

(5) Scullman, Dissertation (Stockholm, 1971); see USIP Report 71-02.

(6) Appelblad, Nilsson, Scullman, PS 7, 65 (1973).

(7) Gingerich, CPL 23, 270 (1973).

PtE: ^aThermochemical value (mass-spectrom.)(1), based on $D_0^0(\text{Te}_2) = 2.68 \text{ eV}$.

(1) See ref. (5) of PS.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(195) Pt ¹ H		$(\mu = 1.00264229) \quad D_0^0 \leq 3.44_0 \text{ eV}^a$							MAY 1975	
IV ($^2\Sigma$) ^b		[2051]	H	8.03	0.40	[4.4] ^c	1.447	IV ← III, R	36504	H (6)
III ($^2\Sigma$) ^b				[9.51]		[3.7]	[1.330]			
II ($^2\Sigma$) ^b				[5.22]		[4.1]	[1.79 ₅]	II ← I, R	30311	H (6)
I ($^2\Sigma$) ^b				[7.13]		[2.8]	[1.536]			
B ($^2\Delta$) _{5/2} (26962)		[1548.18] ^d	Z (80) ^e	6.003 ^{fg}	0.301	[3.15] ^h	1.673 ₆	B ↔ X ₁ , R	26613.91 ^d	Z (1)(3)* (4)(5)
B' ($^2\Phi$) _{7/2} (24218)		[1428.7] ^d	Z (74)	5.758	0.326 ⁱ	[3.6] ^j	1.708 ₈	B' → X ₁ , R	23806.48 ^d	Z (5)*
A ($^2\Delta$) _{5/2} (22311)		1690.6 ^d	Z 55.3 ^k	[5.534] ^l	_m	[3.55] ⁿ	[1.743 ₀]	A ↔ X ₁ , R	21960.59 ^d	Z (1)(2)(3)* (5)
A' ($^2\Delta$) _{3/2} x ₂ ⁺ (19938)		[1500.08] ^d	Z (58)	6.1103 ^o	0.286 ₉	[4.71 ₇] ^p	1.6587 ₉	A' ↔ X ₂ , R	19610.82 ^d	Z (5)*
X ₂ ($^2\Delta$) _{3/2} x ₂ ^q		[2177.31] ^d	Z (43)	7.2784 ^o	0.2029	[2.83 ₄] ^r	1.51987			
X ₁ ($^2\Delta$) _{5/2} 0 ^s		[2294.68] ^d	Z (46)	7.1963	0.1996	[2.61 ₃] ^t	1.52852			
(195) Pt ² H		$(\mu = 1.99350810) \quad D_0^0 \leq 3.59 \text{ eV}^a$							MAY 1975	
B ($^2\Delta$) _{5/2} (26947)		1211.8 ^b	Z 40.3 ^f	3.039 ^{cd}	0.111	0.77 ^e	1.668 ₁	B ← X, R	26703.6 ^b	Z (1)* (2)*
A ($^2\Delta$) _{5/2} (22287)		1198.5 ^b	Z 26.5 ^f	2.935 ^c	0.109	0.76 ^g	1.697 ₄	A ← X, R	22040.5 ^b	Z (1)(2)
X ($^2\Delta$) _{5/2} 0		[1644.3] ^b	Z (23)	3.640	0.071	0.66	1.524 ₂			

Pt¹H: ^aFrom the predissociation in $v=0$ of B ($^2\Delta$)_{5/2}, assuming that X₁ is the ground state.

^bPreliminary data only.

^c $D_1 = 4.9 \times 10^{-4}$.

^dBand origins in the tables for Pt¹H and Pt²H correspond to the energy of J'=0 relative to J''=0. Vibrational constants recalculated accordingly.

^eFrom the corresponding value for Pt²H.

Pt¹H (continued):

^fPerturbations in both $v=0$ and $v=1$.

^gPredissociation above $v=0$, J=12.5, see (5).

$h_{D_1} = 3.94 \times 10^{-4}$.

ⁱPerturbation in $v=1$ at J ≈ 6.5, see (6).

$j_{D_1} = 3.5 \times 10^{-4}$.

$k_{we} = -3.88$ ($v=0, \dots, 3$).

^l Ω -type doubling; for details see (3)(5)(7).

Pt¹H (continued):

^mB₁, B₂, B₃ = 5.244, 4.924, 4.517 (v=3 perturbed for J ≥ 10.5).

ⁿD₁, D₂, D₃(10⁻⁴cm⁻¹) = 3.68, 4.42, 8.8.

^oΩ-type doubling; see (5).

^pD₁ = 6.08 x 10⁻⁴.

^qx₂ ≈ 1320; see (5).

^rD₁ = 2.84 x 10⁻⁴.

^sNot certain that this is the ground state.

^tD₁ = 2.60₇ x 10⁻⁴.

(1) Loginov, OS(Engl. Transl.) 16, 220 (1964).

(2) Neuhaus, Scullman, ZN 19 a, 659 (1964).

(3) Scullman, AF 28, 255 (1964).

(4) Loginov, OS(Engl. Transl.) 20, 88 (1966).

(5) Kaving, Scullman, CJP 49, 2264 (1971).

(6) Scullman, Dissertation (Stockholm, 1971); see USIP Report 71-02.

(7) Kaving, Scullman, PS 2, 33 (1974).

Pt²H: ^aFrom the predissociation in v=2 of B (²Δ)_{5/2}, assuming that X is the ground state. From the value for Pt¹H: D₀⁰ ≤ 3.48₂ eV.

^bSee footnote ^d of Pt¹H.

^cPerturbations.

^dAll lines of the 2-0 band are diffuse.

^eβ_e ≈ + 0.10 x 10⁻⁴.

^fw_ey_e = - 1.5 (v=0, ..., 3).

^gβ_e ≈ + 0.06 x 10⁻⁴.

(1) See ref. (6) of Pt¹H.

(2) See ref. (7) of Pt¹H.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{195}\text{Pt}^{160}$		$\mu = 14.7821844_2$	$D_0^0 = 3.8_2 \text{ eV}^a$							JAN 1976 A
D $^1\Sigma$	(24863)	[567.1] Z	b	[0.33671]	b	[5.19] ^c	[1.8403 ₅]	D→X, R 24722.11 Z		(5)*
A $^1\Sigma$	16995.12	727.07 Z	5.42	0.35385	0.00291	3.2 ₇ ^c	1.7952 ₃	A→X, R 16932.99 Z		(1)(2)(4)*
(X) $^1\Sigma$	0	851.11 Z	4.98	0.38224	0.00283	3.0 ₅ ^c	1.7272 ₆			
$(^{195}\text{Pt}^{218})\text{Si}$		($\mu = 24.4661075$)	$D_0^0 = 5.1_5 \text{ eV}^a$							MAY 1975
$(^{195}\text{Pt}^{232})\text{Th}$		($\mu = 105.946025$)	$D_0^0 = 5.7 \text{ eV}^a$							MAY 1975
$(^{244}\text{Pu}^{19}\text{F}$		($\mu = 17.6263383$)	$D_0^0 = 5.4_6 \text{ eV}^a$							MAY 1975
$(^{226}\text{Ra}^{35})\text{Cl}$		($\mu = 30.2836142$)								JUL 1977
C $^2\Pi$	15386.5	252.9 H	0.72					C→X, R 15384.8 H		(1)
	14782.1	253.8 H	0.71					14780.9		
X $^2\Sigma$	0	256.2 H	0.71							
$(^{85}\text{Rb}_2$		($\mu = 42.455899_5$)	$D_0^0 = 0.49 \text{ eV}^a$		$3.44 < \text{I.P. (eV)}^b \leq 3.95$					JUL 1977 A
		Unidentified features in the absorption spectrum of rubidium vapour at 37270 and 40590 cm^{-1} . (9)								
		Diffuse absorption bands corresponding to van der Waals molecules. (4)								
D	22777.5	40.42 H	0.0745 ^c					D ^d ←X, R 22769.1 H		(3)
C $^1\Pi_u$	20835.1	36.46 H	0.124	Predissociation ^e				C ^d ↔X, ^f R 20824.7 H		(3)
		"Quasicontinuous" emission 16400 - 18500 cm^{-1} . (14)								
B $^1\Pi_u$	14662.6	48.05 H	0.191					B↔X, ^g R 14657.9 H		(2)
A ($^1\Sigma_u^+$)		Unresolved band system 9200 - 12500 cm^{-1} . ^h								(12)(13)(20)
X $^1\Sigma_g^+$	0	57.31 H	0.105					A↔X		
		Mol. beam magn. reson. ⁱ								
$(^{85}\text{Rb}_2^+$				$D_0^0 \geq 0.72 \text{ eV}^b$						JUL 1977
X $^2\Sigma_g^+$	0						(3.94) ^j			

PtO: ^aThermochemical value (mass-spectrom.)(3).

^bLevels with $v > 0$ are perturbed.

^cAlso higher order constants.

(1) Feast, PPS A 63, 549 (1950).

(2) Raziunas, Macur, Katz, JCP 43, 1010 (1965).

(3) Norman, Staley, Bell, JPC 71, 3686 (1967);
AdC No. 72, 101 (1968).

(4) Nilsson, Scullman, Mehendalé, JMS 35, 177 (1970).

(5) Scullman, Sassenberg, Nilsson, CJP 53, 1991 (1975).

PtSi: ^aThermochemical value (mass-spectrom.)(1).

(1) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart,
TFS 66, 809 (1970).

PtTh: ^aThermochemical value (mass-spectrom.)(1).

(1) Gingerich, CPL 23, 270 (1973).

PuF: ^aThermochemical value (mass-spectrom.)(1).

(1) Kent, JACS 90, 5657 (1968).

RaCl: (1) Lagerqvist, AF 6, 141 (1953).

Rb₂, Rb₂⁺:

^aSpectroscopic value (3), extrapolation of vibrational levels in X, C, D.

^bAssociative photoionization of rubidium vapour by atomic line absorption (1)(7)(8).

^c $w_{ey_e} = -0.00144$.

^dLifetime measurements by (11) vary from 61 ns to 14 ns, the former attributed to the D state, the latter to C ¹ Π_u . The two states have also been observed in two-photon ionization of Rb₂ (18).

^eThe state responsible for the partial predissociation

Rb₂, Rb₂⁺ (continued):

($\leq 25\%$) of C ¹ Π_u correlates with the 5p ²P_{3/2} state of Rb (14)(17); see also (16) whose observations of the diffuse and sharp series of Rb in two-photon ionization of rubidium vapour through intermediate continuum states of Rb₂ include only transitions from the ²P_{3/2} component.

^fPolarization studies of the fluorescence spectrum (17)(19) confirm its composition of P and R as well as Q lines, contrary to the conclusions of (14) that it consists of Q line progressions only.

^gMagnetic rotation spectrum (2). The B \rightarrow X (and A \rightarrow X) emission observed by (14) is attributed to atomic recombination of Rb(5²P) and Rb(5²S), the former formed in the predissociation of Rb₂ C ¹ Π_u .

^hInterference by the a ³ Π_u state may be responsible for irregularities in the spectrum at 9900 cm⁻¹ (20).

ⁱ $g_J(^{85}\text{Rb}_2) = 0.00953 \mu_N$ (6); $eqq(^{85}\text{Rb}) = -1.10$ MHz (5).

^jRough estimate based on the analysis of charge exchange cross sections (10). Theoretical calculations predict $r_e = 4.45 \text{ \AA}$ (15).

(1) Lawrence, Edlefsen, PR 34, 233 (1929).

(2) Kusch, PR 42, 218 (1936).

(3) Tsi-Ze, San-Tsiang, PR 52, 91 (1937).

(4) Tsi-Ze, Shang-Yi, JP(Paris) 2, 169 (1938).

(5) Logan, Cote, Kusch, PR 86, 280 (1952).

(6) Brooks, Anderson, Ramsey, PRL 10, 441 (1963); PR A 136,
(7) Lee, Mahan, JCP 42, 2893 (1965). | 62, (1964).

(8) Hudson, JCP 43, 1790 (1965).

(9) Creek, Marr, JQSRT 8, 1431 (1968).

(10) Olson, PR 187, 153 (1969).

(11) Baumgartner, Demtröder, Stock, ZP 232, 462 (1970).

(continued p. 551)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(85)Rb⁴⁰Ar		$(\mu = 27.1735746) \quad D_e^0 = (0.0054) \text{ eV}^a$ Green emission "bands" near the Rb 6s-5s and 4d-5s forbidden transitions (8); similar features observed in absorption (2). Potential curves for all four states have been constructed from studies of the far-wing emission spectra of the Rb resonance lines (4)(5). Near-wing intensities have been measured by (7). Only the A 2Π curves have distinct potential wells with $D_e \approx 330 \text{ cm}^{-1}$ and $r_e \approx 3.35 \text{ \AA}$.								JUL 1977
B $2\Sigma^+$ A $2\Pi_{3/2}$ A $2\Pi_{1/2}$ X $2\Sigma^+$	0	b				(5.2) ^a				
⁸⁵Rb⁷⁹Br		$\mu = 40.902717_4 \quad D_0^0 = 3.9_0 \text{ eV}^a \quad \text{I.P.} = 7.7_5 \text{ eV}^b$ Absorption continua with maxima at 35700, 38800, 46700 cm^{-1} . ^c Diffuse absorption (fluctuation) bands 26600 - 32100 cm^{-1} ; the chemiluminescence spectrum consists of a long lower-state vibrational progression 19000 - 25000 cm^{-1} . 169.46 ^e 0.463 ^e 0.04752798 0.00018596 ^f 1.4959 2.94474 ₄						A ^d ↔X Microwave sp. ^g		JUL 1977 (1)(2)(7) (2)(10) (3)(6)(14)
A X $1\Sigma^+$	0									
(85)Rb(⁷⁹)Br⁺		$D_0^0 = 0.3_3 \text{ eV}^h$ Ionization from the metal 4p shell. ^j Ionization from the halogen 4p shell.								JUL 1977
(D) (116200) _i 114400 _i 111800 _i (109700) (C) 106700 _i (104300) A ($\frac{1}{2}$) 3630 _i X ($\frac{3}{2}, \frac{1}{2}$) 0 _i										

Rb₂, Rb₂⁺ (continued):

- (12) Sorokin, Lankard, JCP 55, 3810 (1971).
- (13) Kostin, Khodovoi, BASPS 37 (10), 69 (1973).
- (14) Brom, Broida, JCP 61, 982 (1974).
- (15) Bellomonte, Cavaliere, Ferrante, JCP 61, 3225 (1974).
- (16) Collins, Curry, Johnson, Mirza, Chellehmalzadeh, Anderson, PR A 14, 1662 (1976).
- (17) Feldman, Zare, CP 15, 415 (1976).
- (18) Granneman, Klewer, Nygaard, Van der Wiel, JP B 2,
- (19) Tam, Happer, JCP 64, 4337 (1976). | 865, (1976).
- (20) Drummond, Schlie, JCP 65, 2116 (1976).

RbAr: ^aSee (1)(3).

^bAn average value $\bar{f} = 3.5 \times 10^{-6} \text{ cm}^{-1}$ for the spin-rotation interaction constant has been derived from relaxation measurements on optically polarized Rb atoms in Ar (6).

- (1) Baylis, JCP 51, 2665 (1969).
- (2) Besombes, Granier, Granier, OC 1, 161 (1969).
- (3) Nikiforov, Shcherba, OS(Engl. Transl.) 32, 567 (1972).
- (4) Drummond, Gallagher, JCP 60, 3426 (1974).
- (5) Carrington, Gallagher, PR A 10, 1464 (1974).
- (6) Bouchiat, Brossel, Mora, Pottier, JP(Paris) 36, 1075 (1975).
- (7) Ottinger, Scheps, York, Gallagher, PR A 11, 1815
- (8) Tam, Moe, Park, Happer, PRL 35, 85 (1975) | (1975).

RbBr, RbBr⁺:

^aThermochem. value (4); 3.98 eV by flame photometry (5).

^bOnset of the photoelectron spectrum (11), vertical transition at 8.17 eV.

RbBr, RbBr⁺ (continued):

^cAlso observed in the electron energy loss spectrum (8), additional peaks at 7.4, 16.3, 19.8 eV. (7) give absorption cross sections from 30300 to 50000 cm⁻¹.

^dThere is no conclusive evidence yet for the identity of the upper states observed in the absorption and emission sp..

^eCalculated from the rotational constants (6).

^f $\gamma_e = + 2.14 \times 10^{-7}$ (14).

$\epsilon_{eqQ}(^{85}\text{Rb}) = -47.2_0 + 0.28(v + \frac{1}{2}) \text{ MHz}$
 $\epsilon_{eqQ}(^{79}\text{Br}) = + 3.0_8 + 0.75(v + \frac{1}{2}) \text{ MHz}$ } (14);

$\mu_{el} = 10.8_6 \text{ D}$ [molecular beam electric deflection (13)].

^hFrom D₀⁰(RbBr), I.P.(Rb), and I.P.(RbBr).

ⁱFrom the maxima of the photoelectron peaks (11)(12); see also (9).

^jThe complexity of the metal 4p photoelectron spectrum is tentatively attributed to configuration interaction (12).

- (1) Müller, AP(Leipzig) 82, 39 (1927).
- (2) Barrow, Caunt, PRS A 219, 120 (1953).
- (3) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (4) Brewer, Brackett, CREV 61, 425 (1961).
- (5) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (6) Rusk, Gordy, PR 127, 817 (1962).
- (7) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (8) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (9) Goodman, Allen, Cusachs, Schweitzer, JESRP 3, 289 (1974).
- (10) Oldenberg, Gole, Zare, JCP 60, 4032 (1974).
- (11) Potts, Williams, Price, PRS A 341, 147 (1974).
- (12) Potts, Williams, JCS FT II 72, 1892 (1976).
- (13) Story, Hebert, JCP 64, 855 (1976).
- (14) Tiemann, Hölzer, Hoeft, ZN 32 a, 123 (1977).

RbCl, RbCl⁺:

^aThermochem. value (7); flame photom. value 4.40 eV (8).

^bOnset of a broad unresolved photoelectron peak with maximum at 8.74 eV (14)(16).

^cAdditional peaks in the electron energy loss spectrum at 7.8, 15.5, 19.0, 23.0 eV (12). (11) give absorption cross sections from 34000 to 50000 cm⁻¹.

^dSee ^d of RbBr.

^eFrom the IR spectrum (6). From the rotational constants (9) calculate $\omega_e = 233.34$, $\omega_e x_e = 0.856$.

^f $r_e = +7.0 \times 10^{-7}$.

^g $\beta_e = +2.3 \times 10^{-11}$.

$\left. \begin{aligned} h_{\text{eqQ}}(^{85}\text{Rb}) &= -52.675 + 0.38 \nu \text{ MHz} \\ h_{\text{eqQ}}(^{35}\text{Cl}) &= +0.774 - 0.155 \nu \text{ MHz} \end{aligned} \right\} \nu = 0, 1, 2 \text{ (5);}$

for constants of ⁸⁷Rb³⁵Cl see (3)(5).

ⁱ $\mu_{\text{el}}[D] = 10.483 + 0.054(\nu + \frac{1}{2})$, $\nu = 0, 1, 2$.

^j $g_J = (-)0.018_3 \mu_N$.

^kFrom D₀(RbCl) and the ionization potentials of Rb and RbCl.

^lFrom maxima of the photoelectron spectrum (16)(17); the halogen 3p spectrum is unresolved. See also ^j of RbBr⁺.

(1) Müller, AP(Leipzig) 82, 39 (1927).

(2) Sommermeyer, ZP 56, 548 (1929).

(3) Bolef, Zeiger, PR 85, 799 (1952).

(4) Barrow, Caunt, PRS A 212, 120 (1953).

(5) Trischka, Braunstein, PR 26, 968 (1954).

(6) Rice, Klemperer, JCP 27, 573 (1957).

(7) Brewer, Brackett, CREV 61, 425 (1961).

(8) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(9) Clouser, Gordy, PR A 134, 863 (1964).

(10) Mehran, Brooks, Ramsey, PR 141, 93 (1966).

RbCl, RbCl⁺ (continued):

(11) Davidovits, Brodhead, JCP 46, 2968 (1967).

(12) Geiger, Pfeiffer, ZP 208, 105 (1968).

(13) Hebert, Lovas, Melendres, Hollowell, Story, Street, JCP 48, 2824 (1968).

(14) Goodman, Allen, Cusachs, Schweitzer, JESRP 3, 289

(15) Oldenborg, Gole, Zare, JCP 60, 4032 (1974). | (1974).

(16) Potts, Williams, Price, PRS A 341, 147 (1974).

(17) Potts, Williams, JCS FT II 72, 1892 (1976).

RbCs: (1) Loomis, Kusch, PR 46, 292 (1934).

(2) Kusch, PR 42, 218 (1936).

(3) Granneman, Klewer, Nygaard, Van der Wiel, JP B 9, 865 (1976).

RbF: ^aThermochemical value (6); flame photometry gives 5.2 eV (7).

^bThe electron energy loss spectrum has peaks at 4.9, 8.2, 9.4, 14.8, 18.4, 19.7, 21.0 eV (14).

^cFrom the IR spectrum (13); good agreement with $\omega_e = 373.27$ and $\omega_e x_e = 1.80$ as calculated from the rot. constants (8).

^d $r_e = +3.30 \times 10^{-6}$. (5)(8) give constants for ⁸⁷RbF.

^e $\beta_e = -0.003_7 \times 10^{-7}$ (8).

^f $\mu_{\text{el}}[D] = 8.5131 + 0.0665_0(\nu + \frac{1}{2}) + 0.0002_6(\nu + \frac{1}{2})^2$, $\nu = 0, 1, 2$ (12) (15); $\text{eqQ}(^{85}\text{Rb})[\text{MHz}] = -70.739 + 0.797_5(\nu + \frac{1}{2}) - 0.005_3(\nu + \frac{1}{2})^2$, $\nu = 0 \dots 4$ (10)(11)(12).

^g(17) give constants for ⁸⁷RbF (eqQ, μ_{el} , g_J , etc.).

^h $g_J = (-)0.044_1 \mu_N$ (9); somewhat different values by (12) for $\nu = 0$ (-0.05470) and $\nu = 1$ (-0.05455).

(1) Caunt, Barrow, Nature 164, 753 (1949).

(2) Hughes, Grabner, PR 72, 314 (1950).

(continued p. 555)

RbF (continued):

- (3) Bolef, Zeiger, PR 85, 799 (1952).
- (4) Barrow, Caunt, PRS A 219, 120 (1953).
- (5) Lew, Morris, Geiger, Eisinger, CJP 36, 171 (1958);
Lew, CJP 42, 1004 (1964) (erratum).
- (6) Brewer, Brackett, CRev 61, 425 (1961).
- (7) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (8) Veazey, Gordy, PR A 138, 1303 (1965).
- (9) Mehran, Brooks, Ramsey, PR 141, 93 (1966).
- (10) Zorn, English, Dickinson, Stephenson, JCP 45, 3731
- (11) Bonczyk, Hughes, PR 161, 15 (1967). | (1966).
- (12) Gräff, Schönwasser, Tonutti, ZP 199, 157 (1967).
- (13) Baikov, Vasilevskii, OS(Engl. Transl.) 22, 198
- (14) Geiger, Pfeiffer, ZP 208, 105 (1968). | (1967).
- (15) Hebert, Lovas, Melendres, Hollowell, Story, Street,
JCP 48, 2824 (1968).
- (16) Matcha, JCP 53, 4490 (1970).
- (17) Heitbaum, Schönwasser, ZN 27 a, 92 (1972).

Rb¹H, Rb²H:

$$\begin{aligned} &^a w_e y_e = -0.25_3, w_e z_e = +0.0030 (v \leq 9). \\ &^b -0.0054(v + \frac{1}{2})^2 + 0.00016_2(v + \frac{1}{2})^3 (v \leq 9). \\ &^c \beta_e \approx -0.026 \times 10^{-4}. \\ &^d w_e y_e = +0.082. \\ &^e y_e = +0.0003. \\ &^f \beta_e \approx -0.01_3 \times 10^{-4}. \end{aligned}$$

- (1) Gaydon, Pearse, PRS A 173, 28 (1939).
- (2) Bartky, JMS 21, 1 (1966).

RbHe: ^aPseudopotential calculations of (1), corrected values quoted by (7). According to (7) the rotationless ground state potential supports one bound level, and a single

RbHe (continued):

quasibound level exists for N=1. The quasibound state has a natural lifetime of 0.6 ns [electron spin relaxation study of optically pumped Rb (5)].

- (1) Baylis, JCP 51, 2665 (1969).
- (2) Besombes, Granier, Granier, OC 1, 161 (1969).
- (3) Drummond, Gallagher, JCP 60, 3426 (1974).
- (4) Tam, Moe, Park, Happer, PRL 35, 85 (1975).
- (5) Franz, Volk, PRL 35, 1704 (1975).
- (6) Ottinger, Scheps, York, Gallagher, PR A 11, 1815 (1975).
- (7) Kiehl, PL A 56, 82 (1976).

RbI, RbI⁺:

- ^aThermochemical value (4), 3.52 eV by flame photometry (5).
- ^bOnset of the first photoelectron peak with maximum at 7.51 eV (11).
- ^cAdditional peaks in the electron energy loss spectrum at 6.4, 15.6, 19.2 eV (8). (7) give absorption cross sections from 26000 to 50000 cm⁻¹.
- ^dSee ^d of RbBr.
- ^eCalculated from the rotational constants (6).
- ^f $y_e = +1.18 \times 10^{-7}$.
- ^g $\beta_e = +0.005_3 \times 10^{-9}$.
- ^h $eqQ(^{85}\text{Rb}) = -40.4_0 \text{ MHz}$, $eqQ(^{127}\text{I}) = -59.8_9 \text{ MHz}$, both for $v=0$ (14). $\mu_{el} = 11.4_8 \text{ D}$ [electric deflection method (13)].
- ⁱ $D_0^0(\text{RbI}) + \text{I.P.}(\text{Rb}) - \text{I.P.}(\text{RbI})$.
- ^jFrom maxima of the photoelectron peaks (9)(11)(12). See also ^j of RbBr⁺.

- (1) Schmidt-Ott, ZP 69, 724 (1931).
 - (2) See ref. (4) of RbF.
 - (3) Honig, Mandel, Stitch, Townes, PR 96, 629 (1954).
- (continued p. 557)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(85)Rb(84)Kr										
		$(\mu = 42.204344_4)$		$D_e^0 = 0.0091 \text{ eV}^a$						JUL 1977
Theoretical potential energy curves correlated with Rb 5^2D , 7^2S , and 4^2F (7). Green emission "bands" near the Rb 6s-5s and 4d-5s forbidden transitions (11); similar features in absorption (3).										
B $2\Sigma^+$	0	}	Potential energy curves for all four states have been constructed from studies of the far-wing emission spectra of the Rb resonance lines (8)(9); near-wing intensities measured by (10). Only the Π curves have deep potential wells with $D_e \approx 420 \text{ cm}^{-1}$ and $r_e \approx 3.5 \text{ \AA}$.							
A $2\Pi_{3/2}$										
A $2\Pi_{1/2}$										
X $2\Sigma^+$										
				b				5.29 ^a		
(85)Rb(20)Ne										
		$(\mu = 16.1823211)$		$D_e^0 = (0.00015) \text{ eV}^a$						JUL 1977
Green emission "bands" near the Rb 6s-5s and 4d-5s forbidden transitions (6); similar features in absorption (2).										
B $2\Sigma^+$	0	}	Far-wing emission spectra of the Rb resonance lines studied by (3)(4), near-wing spectra by (5). The derived 2Π potential curves are attractive with $D_e \approx 150 \text{ cm}^{-1}$ and $r_e \approx 3.4 \text{ \AA}$.							
A $2\Pi_{3/2}$										
A $2\Pi_{1/2}$										
X $2\Sigma^+$										
								(7.8) ^a		
(85)Rb¹⁶O										
		$(\mu = 13.4595306_4)$								JUL 1977
A $2\Pi_{1/2}$	(606) ^a	(389) ^a						(2.41) ^a		
X $2\Sigma^+$	0	(433) ^a						(2.28) ^a		
(85)Rb(132)Xe										
		$(\mu = 51.657726_1)$		$D_e^0 = (0.0134) \text{ eV}^a$						JUL 1977
Green emission "bands" near the Rb 6s-5s and 4d-5s forbidden transitions (8); similar features in absorption (2).										
B $2\Sigma^+$	0	}	Potential curves for all four states have been constructed from the study of the far-wing emission spectra of the Rb resonance lines (4)(6); near-wing intensities measured by (7). B 2Σ is repulsive, A 2Π attractive with $D_e \approx 650 \text{ cm}^{-1}$ and $r_e \approx 3.43 \text{ \AA}$. Teratomic recombination in A $2\Pi_{1/2}$ (5)(9).							
A $2\Pi_{3/2}$										
A $2\Pi_{1/2}$										
X $2\Sigma^+$										
				b				(4.97) ^a		

RbI, RbI⁺ (continued):

- (4) Brewer, Brackett, CRev 61, 425 (1961).
- (5) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (6) Rusk, Gordy, PR 127, 817 (1962).
- (7) Davidovits, Brodhead, JCP 46, 2968 (1967).
- (8) Geiger, Pfeiffer, ZP 208, 105 (1968).
- (9) Goodman, Allen, Cusachs, Schweitzer, JESRP 3, 289 (1974).
- (10) Oldenborg, Gole, Zare, JCP 60, 4032 (1974).
- (11) Potts, Williams, Price, PRS A 341, 147 (1974).
- (12) Potts, Williams, JCS FT II 72, 1892 (1976).
- (13) Story, Hebert, JCP 64, 855 (1976).
- (14) Tiemann, Hoeft, ZN 31 a, 236 (1976).

RbKr: ^aFrom atomic scattering data (1), see also (2)(6).

^bThe existence of Rb-rare-gas van der Waals molecules has been shown in relaxation experiments on optically polarized Rb atoms; see e.g. (4)(5). Average values for the spin-rotation interaction have been derived from these observations: $\bar{\gamma} = 0.0000216$ for RbKr and $\bar{\gamma} \approx 0.00005_2$ for RbXe.

- (1) Buck, Pauly, ZP 208, 390 (1968).
- (2) Baylis, JCP 51, 2665 (1969).
- (3) Besombes, Granier, Granier, OC 1, 161 (1969).
- (4) Bouchiat, Brossel, Pottier, JCP 56, 3703 (1972).
- (5) Bouchiat, Pottier, JP(Paris) 33, 213 (1972).
- (6) Nikiforov, Shcherba, OS(Engl. Transl.) 32, 567 (1972).
- (7) Pascale, Vandeplanque, JCP 60, 2278 (1974).
- (8) Drummond, Gallagher, JCP 60, 3426 (1974).
- (9) Carrington, Gallagher, PR A 10, 1464 (1974).
- (10) Ottinger, Scheps, York, Gallagher, PR A 11, 1815 (1975).
- (11) Tam, Moe, Park, Happer, PRL 35, 85 (1975).

RbNe: ^aPseudopotential calculations (1).

- (1) See ref. (2) of RbKr.
- (2) See ref. (3) of RbKr.
- (3) See ref. (8) of RbKr.
- (4) See ref. (9) of RbKr.
- (5) See ref. (10) of RbKr.
- (6) See ref. (11) of RbKr.

RbO: ^aAb initio calculations (2); experimental evidence for a ² Σ ground state comes from the ESR spectrum of matrix isolated ⁸⁷RbO (1).

- (1) Lindsay, Herschbach, Kwiram, JCP 60, 315 (1974).
- (2) So, Richards, CPL 32, 227 (1975).

RbXe: ^aPseudopotential calculations (1); see also (3)(4).
^bSee ^b of RbKr.

- (1) See ref. (2) of RbKr.
- (2) See ref. (3) of RbKr.
- (3) See ref. (6) of RbKr.
- (4) See ref. (8) of RbKr.
- (5) Carrington, Gallagher, JCP 60, 3436 (1974).
- (6) See ref. (9) of RbKr.
- (7) See ref. (10) of RbKr.
- (8) See ref. (11) of RbKr.
- (9) Scheps, Gallagher, JCP 65, 859 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{187}\text{Re}^{16}\text{O}) ?$		$(\mu = 14.7343266_2)$ Mostly R shaded band heads in the emission spectrum from 11500 to 17400 cm^{-1} . No analysis.							MAY 1975 (1)* (2)	
$^{103}\text{Rh}_2$		$\mu = 51.452756_0$ $D_0^0 = 2.9_2 \text{ eV}^a$							MAY 1975	
$^{103}\text{Rh}^{(11)}\text{B}$		$(\mu = 9.9453102_6)$ $D_0^0 = 4.8_9 \text{ eV}^a$							MAY 1975	
$^{103}\text{Rh}^{12}\text{C}$		$\mu = 10.7467964_1$ $D_0^0 = 6.01 \text{ eV}^a$ Additional systems observed in matrix absorption.							MAY 1975 A	
D $2\Sigma(-)$ (21756)		(782) ^b		(0.482) ^{bc}		(1.80 ₄)			(5)	
C $2\Sigma(+)$ 21439.2		927.8 ^d Z	13.7 ₃	0.5510 ^{de}	0.0060	(1.0)	1.687 ₃	C ← X, R 21376.0 ^d Z	(2) (1)(2)* (5)	
B $2\Sigma(+)$		[0.5067] ^{fg}		(0.8)		[1.759 ₅]		B ← X, R 21361.0 ^f Z	(1)(2)(5)	
A $2\Pi_r$ 10242.75 ^h		939.12 Z	5.48 ⁱ	0.57149	0.00428	0.832 ^k	1.655 ₄	A ↔ X, R 10187.24 ^m Z	(4)(5)	
X $2\Sigma(+)$ 9462.94		949.41 Z	5.357	0.57329 ^j	0.00426	0.826 ^l		9412.60 ^m Z		
	0	1049.87 Z	4.937	0.6027 ⁿ	0.00396	0.78 ₃ ^o	1.613 ₃	ESR sp. ^p		
$^{103}\text{Rh}^{16}\text{O}$		$\mu = 13.8432212_7$ $D_0^0 = 4.2 \text{ eV}^a$ Unclassified R shaded emission bands in the region 15150 - 17050 cm^{-1} .							MAY 1975 (2)	
$^{103}\text{Rh}^{(28)}\text{Si}$		$(\mu = 21.9966876)$ $D_0^0 = 4.0_5 \text{ eV}^a$							MAY 1975	
$^{103}\text{Rh}^{(48)}\text{Ti}$		$(\mu = 32.707955_2)$ $D_0^0 = 4.0_1 \text{ eV}^a$							MAY 1975	

ReO: (1) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
(2) Raziunas, Macur, Katz, JCP 43, 1010 (1965).

Rh₂: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1) Gingerich, Cocke, CC (1972), 536.
(2) Cocke, Gingerich, JCP 60, 1958 (1974).

RhB: ^aThermochemical value (mass-spectrom.)(1).

- (1) Vander Auwera-Mahieu, Peeters, McIntyre, Drowart, TFS 66, 809 (1970).

RhC: ^aThermochemical value (mass-spectrom.)(3)(6).

^bVibrational numbering uncertain. All information based on perturbations in C ²Σ⁽⁺⁾.

^cSpin-splitting constant $\gamma \approx -1.6$.

^dStrong perturbations produced by interaction with B ²Σ⁽⁺⁾, and weaker perturbations produced by D ²Σ⁽⁻⁾.

The constants in the table are deperturbed values. The observed origin of the 0-0 band is at 21452.0 cm⁻¹.

^eSpin-splitting constant $\gamma = -0.03$.

^fVibrational numbering uncertain. Strong interaction with v=0 of C ²Σ⁽⁺⁾. The constants in the table are deperturbed values. The observed band origin is at 21285.0 cm⁻¹.

^gSpin-splitting constant $\gamma = +1.00$.

^hA_v = + 781.07 - 10.50(v+½); also J-dependent terms.

ⁱw_ey_e = + 0.021.

^jΛ-type doubling in ²Π_{1/2}:

Δv_{fe} = (+)[0.0177 + 0.0016(v+½)](J+½).

^kβ_e = + 0.0032 x 10⁻⁶.

^lβ_e = - 0.0019 x 10⁻⁶.

^mJ'=0 relative to N'=0.

RhC (continued):

ⁿSpin-splitting constant $\gamma = -0.065$.

^oβ_e = + 0.012 x 10⁻⁶.

^pIn rare gas matrices at 4 K (5).

- (1) Lagerqvist, Neuhaus, Scullman, ZN 20 a, 751 (1965).

- (2) Lagerqvist, Scullman, AF 32, 479 (1966).

- (3) Vander Auwera-Mahieu, Drowart, CPL 1, 311 (1967).

- (4) Kaving, Scullman, JMS 32, 475 (1969).

- (5) Brom, Graham, Weltner, JCP 52, 4116 (1972).

- (6) Cocke, Gingerich, JCP 52, 3654 (1972); 60, 1958 (1974).

RhO: ^aThermochemical value (mass-spectrom.)(1).

- (1) Norman, Staley, Bell, JPC 68, 662 (1964); AdC No. 72, 101 (1968).

- (2) See ref. (2) of ReO.

RhSi: ^aThermochemical value (mass-spectrom.)(1).

- (1) See ref. (1) of RhB.

RhTi: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1)(2) See ref. (1)(2), resp., of Rh₂.

(Sub-) system	ν_e	w_e'	$w_e'x_e'$	B_e'	α_e'	D_e'	r_e'			References and Remarks
		w_e''	$w_e''x_e''$	B_e''	α_e''	D_e'' (10^{-7}cm^{-1})	r_e'' (\AA)	$\Omega' \leftrightarrow \Omega''$	ν_{00}	
$(^{102}\text{Ru}^{(11)}\text{B})$		$(\mu = 9.9358762_1) \quad D_0^0 = 4.6_0 \text{ eV}^a$								MAY 1975
$^{102}\text{Ru}^{12}\text{C}$		$\mu = 10.73578136 \quad D_0^0 = 6.6_8 \text{ eV}^a$								MAY 1975
XI		Constants for $v=1$:		0.513 ₃ [0.587 ₅]		9.7 [7.5]	1.749 [1.635]	\leftarrow	R 23802.00 ^b Z	(5) P and R br.
X	23299	[743.25] Z		0.5234	0.0069	[9.5] ^c	1.732 ₁	$4 \leftarrow 4,^d$	R 23152.00 Z	(3)(5)* P and R br.
		1038.8 Z	4.6 ₄	0.5878	0.0036	8.3	1.634 ₄			
IX	22925	[775.25] ^e Z		[0.5273]	0.0077 ^e	[10]	[1.725 ₆]	\leftarrow	R 22803.25 Z	(3)(5) P and R br.
		[1018] H		[0.588 ₅]		[7.5]	[1.633]			
VIII		0-0 sequence only.		[0.5637] [0.5882]		[9.6] [8.9]	[1.669 ₀] [1.633 ₉]	\rightarrow	R 15344.82 Z	(4) P, Q, R br.
VII	13862.6 ₄	954.5 ₆ Z	5.39	0.5702	0.0043	9.0 ^f	1.659 ₅	$4 \leftrightarrow 3,$	R 13820.19 Z	(4)* (5) P, Q ^g , R br.
		1039.1 ₄ Z	4.7 ₅	0.5882	0.0040	7.7	1.633 ₉			
VI	13353	[962] H		[0.5701]		[10.2]	[1.659 ₆]	\rightarrow	R 13312.69 Z	(4) P, Q, R br.
		[1043] H		[0.5887]		[9.6]	[1.633 ₂]			
V	13328	[949] H		[0.569 ₇]		[9.6]	[1.660]	\rightarrow	R 13286.43 Z	(4) P, Q, R br.
		[1032] H		[0.5882]		[8.6]	[1.633 ₉]			
IV	13138	960 H	3	[0.5698]		[8.4]	[1.660 ₀]	$2 \rightarrow 1,$	R 13094.87 Z	(4) P, Q, R br.
		1048 H	5.5	[0.5879] ^h		[8.1]	[1.634 ₃]			
III	12913	[944] H		[0.5691]		[9.4]	[1.661 ₁]	\rightarrow	R 12875.23 Z	(4) P, Q, R br.
		[1020] H		[0.5882]		[9.0]	[1.633 ₉]			
II		0-0 sequence only.		[0.5710] [0.5864]		[9.1] [7.8]	[1.658 ₃] [1.636 ₄]	(2) \rightarrow (3),	R 12658.26 Z	(4) P, Q, R br.
I	12664	(950) H		[0.5653]		[7.5]	[1.666 ₆]	\rightarrow	R 12624.28 Z	(4) P, Q, R br.
		(1030) H		[0.5870]		[6.6]	[1.635 ₅]			

RuB: ^aThermochemical value (mass-spectrom.)(1).

(1) See ref. (1) of RhB.

RuC: ^aThermochemical value (mass-spectrom.)(1), revised (2);
(6).

^bOnly 1-0 band analyzed.

^c $D_1 = 8.0 \times 10^{-7}$.

^dIt is possible that the lower state of system X is identical with that of system VII. In this case, $\Omega' = \Omega'' = 3$.

^eAssignment of 1-0 band not certain. Lower state constants for this band are $B_0'' = 0.5869$, $D_0'' = 7.0 \times 10^{-7}$.

^f $\beta_e = -0.3 \times 10^{-7}$.

^gPerturbations.

^hThe Ω -type doubling in the 0-0 band, $\Delta v \approx 0.00010_3 \times J(J+1)$, is believed to arise in the lower state.

RuC (continued):

(1) McIntyre, Vander Auwera-Mahieu, Drowart, TFS 64, 3006 (1968).

(2) See ref. (1) of RhB.

(3) Scullman, Dissertation (Stockholm, 1971); see USIP Report 71-02.

(4) Scullman, Thelin, PS 3, 19 (1971).

(5) Scullman, Thelin, PS 5, 201 (1972).

(6) Gingerich, CPL 25, 523 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
$^{102}\text{Ru}^{16}\text{O}$		$\mu = 13.8249497_5$ $D_0^0 = 5.3 \text{ eV}^a$ Additional unclassified emission bands in the region $15500 - 17200 \text{ cm}^{-1}$.								MAY 1975	
B_3	$a_3 + 18121.4$	792.9	H	4.1	0.3818	0.0025	4	1.787 ₁	$B_3 \rightarrow A_3,^b$ R	18086.2 Z	(1)(3)*
B_2	$(n=3) a_2 + 18101$	[783]	H		[0.382] ^c		[6] ^c	[1.78 ₇]	$B_2 \rightarrow A_2,^b$ R	18065.1 Z	(1)(3)*
B_1					[(0.384)]			[(1.78)]	$B_1 \rightarrow A_1,^b$ R	18024 Z	(1)(3)
A_3	a_3^d	863.5	H	4.6	0.4137	0.0028	3	1.716 ₈			
A_2	$(n=3) a_2^d$	[855]	H		[0.4144] ^e		[3.9]	[1.715 ₄]			
A_1	a_1^d				[(0.414)]			[(1.72)]			
$(^{102}\text{Ru}^{28})\text{Si}$		$(\mu = 21.9505901)$ $D_0^0 = 4.0_8 \text{ eV}^a$								MAY 1975	
$(^{102}\text{Ru}^{232})\text{Th}$		$(\mu = 70.807681_5)$ $D_0^0 = 6.1 \text{ eV}^a$								MAY 1975	
$^{32}\text{S}_2$		$\mu = 15.9860364$ $D_0^0 = 4.3693 \text{ eV}^a$ I.P. = 9.36 eV^b								JUL 1977	
		Additional progressions and unassigned bands in the absorption spectrum $65700 - 71900 \text{ cm}^{-1}$.								(50)	
F	c (66333) (66229)	[827] ^d	H						$F \leftarrow X,$ 66384 ^d H 66280 ^d H		(36)(50)
E	c (65933) (65829)	[818] ^d	H						$E \leftarrow X,$ 65980 ^d H 65876 ^d H		(36)(50)
j		Only $v=0$ observed.							$j \rightarrow (b),^e$ V	56077.7 H	(25)*
i		[785.0]	H						$i \rightarrow (b),^e$ V	55099.3 H	(12)*
h		819.6	H	2.70					$h \rightarrow (b),^e$ V	51461.4 H	(12)*
D	$^3\Pi_{u,r}$ 58978.7 58691.7 58518.3	793.8	H	4.00	[0.3073] [0.3066] [0.3059]		[1.85]	[1.854 ₆]	$D \leftrightarrow X,$ V	59012.50 Z 58725.47 Z 58552.05 Z	(8)* (12) (31)
g	$^1\Delta_u$ x + 52187.7	816.0	H	2.70	[0.3210]		(2.0)	[1.812 ₅]	$g \leftrightarrow a,^f$ V	52244.66 Z	(12)* (26)
$C'(^3\Sigma_u^-)$		$v=0$ only; system e-X of (12).							$C' \rightarrow X,$ V	56621.6 H	(12)*

- RuO: ^aThermochemical value (mass-spectrom.)(2).
^bR and P branches only.
^cB₁ = 0.381, D₁ = 9 x 10⁻⁷. Perturbations.
^dRelative position of these three states unknown.
^eB₁ = 0.413.
 (1) See ref. (2) of ReO.
 (2) Norman, Staley, Bell, AdC No. 72, 101 (1968).
 (3) Scullman, Thelin, JMS 56, 64 (1975).
- RuSi: ^aThermochemical value (mass-spectrom.)(1).
 (1) See ref. (1) of RhB.
- RuTh: ^aThermochemical value (mass-spectrom.)(1).
 (1) See ref. (6) of RuC.
- S₂: ^aFrom the predissociation limit in B ³Σ_u⁻ assuming dissociation at this limit into ³P₂ + ³P₁ (32). The value given here (35240.2 cm⁻¹) is relative to the lowest existing level in X ³Σ_g⁻(v=0), i.e. J=0, in accordance with the definition of D₀⁰ but at variance with the value given by (32) which refers to a hypothetical level (N=0) of the F₂ component at 23.1 cm⁻¹ above J=0. D₀⁰ = 4.38 eV by photoionization mass-spectrometry (30), 4.4₁ eV from thermal measurements (27). See also (23).

S₂ (continued):

- ^bBy photoionization mass-spectrometry (28)(30).
^cThe two states E and F are believed to be members of two Rydberg series, one converging to X ²Π_{1/2} of S₂⁺ (C,E,...), the other to X ²Π_{3/2} (F,...). The apparent doublet structure of the bands is tentatively attributed to (Ω_C,ω) coupling (36).
^dMeasurements of (50); assignments of higher members of the two progressions appear uncertain.
^eThe lower state(s) of the three systems could be either a or b; see (18)(26). Bands originating from the j level have double heads, all others single heads. No absorption corresponding to these transitions has been reported, although strong absorption from a ¹Δ_g (g←a, f←a) has been seen in the flash photolysis of S₂Cl₂ (28a)(36) and COS (35). (12) use c and c' instead of h and i, respectively.
^fCalled d→x by (12). Observed in absorption in the flash photolysis of S₂Cl₂ (36).

S₂ (continued from p. 565):

- ^bSpin splitting constants λ_v = +11.82 + 0.05(v+½) + 0.0024 x (v+½)², γ_v = -0.00659 - 0.000126(v+½) for v ≤ 27, from (44) who give also data for ³Δ₂; see also (13)(18)(45). From the pure rotational Raman spectrum (46) obtain B₀ = 0.29443.
^cγ_e = -1.8₂ x 10⁻⁶ (18).
^dRaman spectra in solid matrices (37)(47) yield ΔG = 717.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$^{32}\text{S}_2$ (continued)										
C $^3\Sigma_u^-$	55581.7	829.1 ₅	Z	3.3 ₄	0.3219 ^g	0.0013 ₈ ^h	[2.1 ₇]	1.810 ₀	C↔X, V	55633.3 ⁱ Z (3)(8)* (12)(29)*
f $^1\Delta_u$	x+36875.45	438.32	Z	2.70 ^j	0.22704 ^k	0.00178	(2.4 ₃)	2.155 ₁	f↔a, ^l R	36743.53 Z (26)(35)
B' $^3\Pi_{g,i}$	$\begin{cases} - \\ z+(14504) \\ z+(14295) \end{cases}$	$\begin{cases} - \\ [533.7]^m \\ - \end{cases}$	$\begin{cases} - \\ (Z) \end{cases}$	$\begin{cases} - \\ [0.244_1]^n \\ [0.243_5]^n \end{cases}$	$\begin{cases} - \\ - \\ - \end{cases}$	$\begin{cases} - \\ - \\ - \end{cases}$	$\begin{cases} - \\ - \\ - \end{cases}$	$\begin{cases} - \\ - \\ - \end{cases}$	B'→A, V	$\begin{cases} - \\ 13451.9_5^o Z \\ 13320.6_4^o Z \end{cases}$ (16)(24) (49)*
B $^3\Sigma_u^-$	31835	434.0 ^p		2.75 ^p	0.2239 ^{pqr}	0.0023 ^p	[2.4] ^p	2.170	B ^s ↔X, ^t R	$\begin{cases} - \\ 14144.3_7 Z \\ 14318.0_7 Z \end{cases}$ (10)(16) (24)(48)*
A $^3\Sigma_u^+$	$\begin{cases} 0_u^- & z+1078^v \\ 1_u & z+1000.4_9 \end{cases}$	$\begin{cases} 482.7_5 \\ 482.1_5 \end{cases}$	$\begin{cases} Z \\ Z \end{cases}$	$\begin{cases} 2.5_8 \\ 2.5_6 \end{cases}$	$\begin{cases} 0.230_1 \\ 0.225_9^w \end{cases}$	$\begin{cases} 0.0021 \\ 0.0014 \end{cases}$		$\begin{cases} 2.141 \\ 2.161 \end{cases}$		
A' $^3\Delta_{u,i}$	$\begin{cases} - \\ z+383 \\ z^x \end{cases}$	$\begin{cases} - \\ 488.1_6 \\ 488.2_5 \end{cases}$	$\begin{cases} - \\ Z \\ Z \end{cases}$	$\begin{cases} - \\ 2.5_1 \\ 2.5_2 \end{cases}$	$\begin{cases} - \\ 0.228_5 \\ 0.228_5 \end{cases}$	$\begin{cases} - \\ 0.001_4 \\ 0.001_5 \end{cases}$		$\begin{cases} - \\ 2.148 \end{cases}$		
b $^1\Sigma_g^+$	y	(699.7) ^y		(3.4) ^y						
a $^1\Delta_g$	x ^z	702.35	Z	3.09	0.29262	0.00173	(2.01)	1.8983		
X $^3\Sigma_g^-$	0 ^{a'}	725.65	Z	2.844	0.2954 ₇ ^{b'}	0.001570 ^{c'}	[1.9 ₀]	1.8892	$\begin{cases} \text{Raman sp.}^d \\ \text{EPR and} \\ \text{mol. beam rf sp.} \end{cases}$	(40)(46) (45) (25a)

S_2 (continued):

^gSpin splitting constants $\lambda_0 = -11.6_1$, $\gamma_0 = +0.033$.

^h $\gamma_e = -0.00023$.

ⁱThis number, given or implied by (18)(29), refers presumably to the F_2 levels in both upper and lower state.

^j $\omega_e y_e = -0.005$.

^kBreaking-off in emission above $v'=10$ (20)(22). In absorption (35) bands with $v'=11$ and 12 have been observed, the rotational lines being only very slightly broadened. Predissociation probably into $^3\Delta_u$ from $^3P+^1D$.

^lFirst observed by (4)(15). Vibrational numbering established

S₂ (continued):

by isotope investigations (17)(21).

^mFragments of two V shaded emission bands at $\nu_0 = 13451.9$ and 13985.5 cm^{-1} have been observed by (10) and assigned (18) to a $1\Pi_g \rightarrow 1\Sigma_u^-$ transition later called e \rightarrow c (26). The first band ($B' \approx 0.244$, $B'' \approx 0.229$, predissociated except for low J) is undoubtedly the 0-0 band of the $B' \ 3\Pi_{g1} \rightarrow A' \ 3\Sigma_u^+(0_u^-)$ transition, the second presumably the corresponding 1-0 band since the $\Delta G(\frac{1}{2})$ value agrees fairly well with $\omega_e \approx 500$ as estimated from isotope shift studies (24). However, no emission from levels having $v' > 0$ was reported by other investigators.

ⁿThe last observed levels in emission are $J'=33$ and 15 in $3\Pi_2$ and $3\Pi_1$, respectively; higher levels, and presumably all levels of the unobserved $3\Pi_0$ component, are predissociated.

^oOrigins of the $3\Pi_{2g} \rightarrow 3\Sigma_u^+(1_u)$ and $3\Pi_{1g} \rightarrow 3\Sigma_u^+(0_u^-)$ transitions.

^pVibrational constants from (6), rotational constants from (9). (18) give $B_0 = 0.2235$, $\alpha_e = 0.0018$ (i.e. $B_e = 0.2244$) without mentioning whether this is based on a revised analysis. This state is heavily perturbed by a $3\Pi_u$ state (18); as a result none of the constants are very meaningful.

^qSpin splitting constant $\lambda \approx -4.7$ for $v=0,2,4$ ($v=6,7$ are also inverted) but $+9.5$ for $v=1,3,5$ (43); see P. (18) give $\lambda = +0.05$ for $v=0,1,4$.

^rBreaking-off in emission (at low pressure) above

$$\left. \begin{array}{l} J=61 \\ J=58 \\ J=59 \end{array} \right\} \text{ in } v=8, \text{ and } \left. \begin{array}{l} J=37 \\ J=36 \\ J=35 \end{array} \right\} \text{ in } v=9 \quad \left. \begin{array}{l} (F_1 \text{ component}) \\ (F_2 \text{ component}) \\ (F_3 \text{ component}) \end{array} \right\} (32).$$

These together with similar breaking-off points in $34S_2$ and $32S^{34}S$ yield a predissociation limit at 35636.3 cm^{-1} above $X \ 3\Sigma_g^-(v=0, J=0)$ of $32S_2$. Bands with $v' \geq 10$ are absent in

emission [except at high pressure (1)(2)(11)] and broadened in absorption. Above $v'=18$ there is strongly increased diffuseness indicating a second predissociation (?). Pressure effects on the intensity distribution of the absorption bands (5)(14).

^sLifetime $\tau(v=0...3) = 17 \text{ ns}$ [phase shift method (33)];

$$\tau(v=3, 4) = 19.5 \text{ ns} \text{ [Hanle effect (41)]}.$$

The most recent measurements [single-photon time correlation (51)] give $\tau = 45.0 \text{ ns}$.

^tSecondary heads on the short-wavelength side of the bands are formed by the forbidden T_{R31} branches [(10), see also (39)]. Experimental Franck-Condon factors ($v''=0...25$) from resonance fluorescence series with $v'=3,4$ (42), see also (40). Theoretical Franck-Condon factors (14)(38) [see, however, P]. $32S_2/34S_2$ isotope shifts (34). Absorption in inert gas matrices at low temperature (19).

^uThe observed position of $v'=0$ relative to $X \ 3\Sigma_g^-(v''=0)$ is at 31659 cm^{-1} ; strong vibrational perturbation.

^v $\lambda = -39.0$ (and $\gamma = +0.008$) derived from the observed $F_1(N) - F_2(N)$ splittings (49).

^w $B^+(F_2) - B^-(F_1) = +0.0021$.

^x $\approx 22000 \text{ cm}^{-1}$, very rough estimate based on the fact that the upper state of $B' \rightarrow A'$ is predissociated and, therefore, cannot lie below the dissociation limit $3P + 3P$. A similar value is obtained by extrapolation of the vibrational levels in A' and X to their common limit $3P + 3P$.

^yAssuming that b is the lower state of the three singlet systems originating from h, i, j.

^z(35) estimate $x \approx 4700 \text{ cm}^{-1}$.

^aRefers to the F_2 component.

(continued on p. 563, ref. on p. 567)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{32}\text{S}_2^+$		$\mu = 15.9858993$ $D_0^0 = 5.37$ eV ^a							JUL 1977	
Several additional unresolved photoelectron peaks with vertical I.P.'s of 15.58 ($^2\Pi_u$), 17.73, 18.10, 18.66, 23.33, 25.99 eV (2).										
B	$^2\Sigma_g^-$ 41820	540					(1.98 ₃)			
b	$^4\Sigma_g^-$ 30920	580	All constants obtained by photoelectron spectroscopy (2); data of somewhat lower resolution are given by (1). Internuclear distances derived from Franck-Condon factor analyses of the photoelectron spectra (2).				(1.93 ₆)			
A	$^2\Pi_u$ 22390	530					(2.04 ₂)			
a	$^4\Pi_u$ 17440	600					(2.05 ₈)			
X	$^2\Pi_{g,r}$ 470 0	790					(1.82 ₅)			
$^{32}\text{S}_2^-$		$\mu = 15.9861735$ $D_0^0 = 3.95_5$ eV ^a I.P. = 1.66 ₃ eV ^b							JUL 1977	
A'	$(^2\Pi_u)$ 20220 ^c	364.2 ₅ ^d	2.00	Constants for S_2^- ions dissolved in KI crystals, from spectra studied at 2 K (5)(7); see also (8). Host crystals other than KI lead to somewhat different values.				A' ← X,	20102	(7)
A	20143							A → X',	19452	(5)(8)
X'	$(^2\Pi_{g,i})$ 573 ^c	600.8	3.01					A ↔ X,	20025	(2)(5)(7)(8)
X	0	600.8 ^e	2.16					Raman sp.		(3)(8)
							EPR sp.		(1)	

$$S_2^+: {}^aD_0^0(S_2) + \text{I.P.}(S) - \text{I.P.}(S_2).$$

- (1) Berkowitz, JCP 62, 4074 (1975). | (1975).
 (2) Dyke, Golob, Jonathan, Morris, JCS FT II 71, 1026

$$S_2^-: {}^a\text{From } D_0^0(S_2) \text{ and the electron affinities of } S_2 \text{ and } S.$$

^bFrom laser photodetachment experiments (6).

^cThe splitting is due to the crystal field, not spin-orbit coupling which in the $^2\Pi_g$ state amounts to approximately -420 cm $^{-1}$ (1)(7).

^dThe Raman spectrum of ions pumped into this state by laser irradiation consists of a sharp line shifted by 362 cm $^{-1}$ (4).

S_2^- (continued):

^e(3) predict a gas phase frequency of ~ 550 cm $^{-1}$.

- (1) Vannotti, Morton, PR 161, 282 (1967).
 (2) Rolfe, JCP 49, 4193 (1968).
 (3) Holzer, Murphy, Bernstein, JMS 32, 13 (1969).
 (4) Holzer, Racine, Cipriani, AdRS 1, 393 (1973).
 (5) Ikezawa, Rolfe, JCP 58, 2024 (1973).
 (6) Celotta, Bennett, Hall, JCP 60, 1740 (1974).
 (7) Vella, Rolfe, JCP 61, 41 (1974).
 (8) Sawicki, Fitchen, JCP 65, 4497 (1976).

S₂ (continued):

- (1) Asundi, Nature 127, 93 (1931).
- (2) Asundi, CS 3, 154 (1934).
- (3) Wieland, Wehrli, Miescher, HPA 7, 843 (1934).
- (4) Rosen, Désirant, BSRSL 4, 233 (1935).
- (5) Kondratjew, Olsson, ZP 99, 671 (1936).
- (6) Olsson, Thesis, Stockholm (1938).
- (7) Herzberg, Mundie, JCP 8, 263 (1940).
- (8) Maeder, HPA 21, 411 (1948).
- (9) Ikenoue, SL 9, 79 (1960).
- (10) Meakin, Barrow, CJP 40, 377 (1962).
- (11) Sugden, Demerdache, Nature 195, 596 (1962).
- (12) Tanaka, Ogawa, JCP 36, 726 (1962).
- (13) Barrow, Ketteringham, CJP 41, 419 (1963).
- (14) Herman, Felenbok, JQSRT 3, 247 (1963).
- (15) Haranath, ZP 173, 428 (1963).
- (16) Narasimham, CS 33, 261 (1964).
- (17) Narasimham, Brody, PIAS A 59, 345 (1964).
- (18) Barrow, du Parcq, in "Elemental Sulphur" (ed. Meyer), p. 251, New York Interscience (1965).
- (19) Brewer, Brabson, Meyer, JCP 42, 1385 (1965).
- (20) Asundi, JCP 43, S24 (1965).
- (21) Narasimham, Bhagvat, PIAS A 61, 75 (1965).
- (22) Narasimham, Gopal, CS 34, 454 (1965).
- (23) Drowart, Goldfinger, QR 20, 545 (1966).
- (24) Narasimham, Apparao, Nature 210, 1034 (1966).
- (25) Lakshminarayana, Narasimham, CS 36, 533 (1967).
- (25a) Channappa, Pendlebury, Smith, in "La Structure Hyperfine Magnétique des Atomes et des Molécules" (ed. Moser and Lefebvre), p. 73, éditions du CNRS (Paris, 1967).
- (26) Barrow, du Parcq, JP B 1, 283 (1968).
- (27) Budininkas, Edwards, Wahlbeck, JCP 48, 2859 (1968).
- (28) Berkowitz, Lifshitz, JCP 48, 4346 (1968).
- (28a) Donovan, Husain, Jackson, TFS 64, 1798 (1968).
- (29) Barrow, du Parcq, Ricks, JP B 2, 413 (1969).
- (30) Berkowitz, Chupka, JCP 50, 4245 (1969).
- (31) Ricks, Barrow, JP B 2, 906 (1969).
- (32) Ricks, Barrow, CJP 47, 2423 (1969).
- (33) Smith, JQSRT 9, 1191 (1969).
- (34) Chaudhry, Upadhyaya, Nair, IJPAP 8, 52 (1970).
- (35) Carleer, Colin, JP B 3, 1715 (1970).
- (36) Donovan, Husain, Stevenson, TFS 66, 1 (1970).
- (37) Barletta, Claassen, McBeth, JCP 55, 5409 (1971).
- (38) Smith, Liszt, JQSRT 11, 45 (1971).
- (39) Tatum, Watson, CJP 42, 2693 (1971).
- (40) Yee, Barrow, Rogstad, JCS FT II 68, 1808 (1972).
- (41) Meyer, Crosley, JCP 52, 1933 (1973).
- (42) Meyer, Crosley, JCP 52, 3153 (1973).
- (43) Meyer, Crosley, CJP 51, 2119 (1973).
- (44) Barrow, Yee, APH 35, 239 (1974).
- (45) Wayne, Davies, Thrush, MP 28, 989 (1974).
- (46) Freedman, Jones, Rogstad, JCS FT II 71, 286 (1975).
- (47) Hopkins, Brown, JCP 62, 1598 (1975).
- (48) Narasimham, Sethuraman, Apparao, JMS 59, 142 (1976).
- (49) Narasimham, Apparao, Balasubramanian, JMS 59, 244 (1976).
- (50) Mahajan, Lakshminarayana, Narasimham, IJPAP 14, 488 (1976).
- (51) McGee, Weston, CPL 47, 352 (1977).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-9}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(121,123)Sb₂										
		$(\mu = 60.947907_4) \quad D_0^0 = 3.09 \text{ eV}^a$								JUL 1977
		Fragments of other emission band systems 11900 - 13900 (V shaded), 23800 - 27800, 33300 - 34500 cm^{-1} (R shaded).								(6)
U	(70194)	[272] ^b		Weak diffuse bands.				U \leftarrow X,	70195	(7)
M	(63258)	[152] ^c	H	Three sharp bands.				M \leftarrow X,	63199	H (7)
I	(59142)	[210] ^d	H	Weak system.				I \leftarrow X,	59112	H (7)
G	(53888)	[185] ^e	H					G \leftarrow X, R	53846	H (7)* (10)(11)
E	(48645)	[228] ^f	H	The bands appear diffuse.				E \leftarrow X,	48624	H (7)* (10)
F	44780	226.0 ^g	H	1.17				F \leftarrow X, (R)	44758	H (1)(10)
H	(44329)	[479] ^h	H	Single progression, observed in ¹²¹ Sb ₂ .				H \leftarrow X, V (44433) ^h		H (11)
D	(32087)	[209.6] ⁱ	H					D \leftrightarrow X, R	32057	H (2)(6)
B	0 _u ⁺ 19068.9	218.0 ₈	H	0.53 ₇	$B_2 = 0.044844^j$	$D_2 = 9.2$	$r_2 = 2.4835$	B \leftrightarrow X, R	19043.0	H (3)(4)(8)
A	14991	217.2	H	0.44				A \leftrightarrow X, R	14965	H (3)(4)
X	1 Σ_g^+ 0	269.9 ₈	H	0.58 ₈	$B_2 = 0.050447^j$	$D_2 = 9.5$	$r_2 = 2.3415$			
¹²¹Sb⁷⁵As										
		$\mu = 46.257057_6$								JUL 1977
A	(¹ Π) 27366	[204.7]	H					A \rightarrow X, R	27297.1	H (1)
X	1 Σ^+ 0	343.0	H	0.8						
(121)Sb²⁰⁹Bi										
		$(\mu = 76.592111_7)$								JUL 1977
A	40647 ^a	190.2	H	0.73				A \leftarrow X, R	40632	H (1)*
X	1 Σ^+ 0	220.0	H	0.50						
(121)Sb⁽⁷⁹⁾Br										
		$(\mu = 47.750100_7)$								JUL 1977
		Two emission continua with maxima at 15400 and 19200 cm^{-1} .								(1)(4)
		Strong diffuse absorption bands in the flash photolysis of SbBr ₃ , 41200 - 44200 cm^{-1} . $\Delta G' \approx 340$, $\Delta G'' \approx 258$; analysis seems doubtful.								(2)
C	(³ Π)							C \leftarrow X, V	44220 43269 42265	

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(121)Sb(79)Br (continued)										
B_2	(33740)	201.0	H	0.30				$B_2 \rightarrow X, ^a R$	33719	H (1)(3)
B_1	(32372)	207.6	H	0.85				$B_1 \rightarrow X, ^a R$	32354	H (1)(3)
A	(19749)	215.8	H	0.35				$A \rightarrow X, ^a R$	19736	H (1)(4)
$X_2 ({}^3\Sigma^-) \frac{1}{2}$ $X_1 \quad 0^+$	0	242.7	H	0.56						

Sb₂: ^aThermochemical value (mass-spectrom.)(5)(9).

^b $\Delta G(3/2) = 254$.

^c $\Delta G(3/2) = 149$.

^d $\Delta G(3/2, 5/2) = 216, 217$.

^e $\Delta G(3/2, 5/2) = 195, 205$ (10); (7) give also $\Delta G(7/2) = 196$. Bands of ¹²¹Sb₂ (11).

^f $\Delta G(3/2 \dots 9/2) = 216, 217, 220, 246$ (7) [flash photolysis of SbH₃]; (10) [high temp. abs.] give no assignments.

^g(10) express doubts about the correctness of the analysis.

^h $\Delta G(3/2 \dots 13/2) = 541, 528, 477, 517, 548, 472$. The constants assume $v'=0, v''=2$ for the first b. at 43897 cm^{-1} .

ⁱLevels up to $v'=17$ have been observed; the ΔG values are irregular due to perturbations and vary between 208 and 228. (1) give different assignments and constants.

^jConstants for ^{121,123}Sb₂ from the rotational analysis of the $B \rightarrow X$ 2-2 band by (8) who give also constants for ¹²¹Sb₂ and ¹²³Sb₂.

(1) Nakamura, Shidei, JJP 10, 11 (1935).

(2) Naudé, SAJS 32, 103 (1935).

Sb₂ (continued):

(3) Almy, JPC 41, 47 (1937).

(4) Almy, Schultz, PR 51, 62 (1937).

(5) De Maria, Drowart, Inghram, JCP 31, 1076 (1959).

(6) Mrozowski, Santaram, JOSA 57, 522 (1967).

(7) Donovan, Strachan, TFS 67, 3407 (1971).

(8) Sfeila, Perdigon, Martin, Fémelat, JMS 42, 239 (1972).

(9) Kordis, Gingerich, JCP 58, 5141 (1973).

(10) Topouzkhanian, Sibai, d'Incan, ZN 29 a, 436 (1974).

(11) Sibai, Topouzkhanian, d'Incan, CR B 280, 79 (1975).

SbAs: (1) Yee, Jones, CC (1969), 752.

SbBi: ^a(1) give erroneously 40617.

(1) See ref. (1) of Sb₂.

SbBr: ^aUndecided whether the lower state is X_1 or X_2 .

(1) Singh, Avasthi, IJPAP 1, 197 (1963).

(2) Danon, Chatalic, Deschamps, Pannetier, CR C 269, 1249 (1969).

(3) Avasthi, ZN 26 a, 250 (1971).

(4) Avasthi, Sharma, Sud, ZN 30 a, 695 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(121) Sb^{35}Cl										
$(\mu = 27.1238563)$										
E	(47358)	[(446)]	H					$E \leftarrow X$, V	47394	H (4)
D	(45216)	[436]	H					$D \leftarrow X$, ^a V	45247 ^b	H (4)* (5)
C	(43069)	444	H	3				$C \leftarrow X$, ^a V	43103 ^b	H (2)(4)* (5)
B	(41616)	448	H	4				$B \leftarrow X$, ^a V	41652	H (5)
A_2	(25906)	240.9 ^c	H	0.8 ₅				$A_2 \rightarrow X$, ^a R	25839 ^c	H (1)* (3)
A_1	(22178)	237.5 ^c	H	1.5				$A_1 \rightarrow X$, ^a R	22109 ^c	H (1)* (3)
$b \ 0^+$	12148.7	382.1	H	0.6				$b \rightarrow X_2$, ^d V	12152.4	H ^Q (6)*
$X_2 \ (3\Sigma^-)^1$	816.3 ^f							$b \rightarrow X_1$, ^e V	12958.9	H ^P (6)*
X_1	0	374.7	H	0.6						
(121) Sb^{19}F										
$\mu = 16.4184644 \quad D_0^0 = (4.4) \text{ eV}$										
$C_3 \ 1$	44756.7	[696.2 ₇]	Z	3.0 H		0.2983 ^a	0.0029	(2.2)	1.855 ₃	$C_3 \rightarrow b$, V 31148.9 Z (8)*
										$C_3 \rightarrow a$, V 37983.53 Z (1a)(8)*
										$C_3 \leftrightarrow X_1$, V 44802.6 Z (1a)(2)(8)*
C_2	44310.4	700.9	H	2.8 ₀						$C_2 \rightarrow X_2$, V 43558.2 H (1a)(2)
$A_3 \ 1$	28706.6	411.1	Z	1.67		0.2414	0.0017 ₀	(3.3)	2.062 ₄	$A_3 \rightarrow b$, R 14953.8 ^b (Z) (9)*
										$A_3 \rightarrow a$, R 21788.3 ^b (Z) (1)* (9)*
										$A_3 \rightarrow X_2$, R 27809.7 ^b (Z) (1a)(9)*
$A_2 \ 2$	24788.4	420.3	Z	1.71		0.2411	0.0016 ₅	(3.2)	2.063 ₆	$A_2 \rightarrow a$, R 17874.6 ^c (Z) (9)*
										$A_2 \rightarrow X_2$, R 23896.1 ^c (Z) (1)* (9)*
A_1	22589.4	418.9	H	2.6 ₄						$A_1 \rightarrow X_1$, R 22493.7 H (3)*
$A \ 0^+$	21407.5	416	H	2.1		[0.2385 ₃]		[3.2 ₂]	[2.074 ₇]	$A \rightarrow X_2$, R 20513.0 ^d (Z) (6)(9)*
										$A \rightarrow X_1$, ^e R 21311 (9)
$b \ 1\Sigma^+$	13651.1	615.5	H	2.8		0.2815	0.0025	(2.4)	1.909 ₈	$b \rightarrow X_2$, 12856.1 ₅ Z (7)*
										$b \rightarrow X_1$, 13653.6 ₈ Z (7)*

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{121}\text{Sb}^{19}\text{F}$ (continued)										
a $^1\Delta$	6816.0	616.3	Z 2.7 ₀	0.2806	0.0018 ₇	(2.3)	1.912 ₉			
$X_2(3\Sigma^-)^1$	796.3	612.6	H 2.6 ₁	0.2805 ^f	0.0020	(2.4)	1.913 ₂			
X_1 0^+	0	[605.0]	Z 2.6 ₂ H	0.2792	0.0020	(2.3)	1.917 ₇			

SbCl: ^aIt is not decided whether the lower state is X_1 or X_2 , both of the emission and of the absorption bands.

^bAverage values of constants given by different groups of authors.

^cConstants of (3) who has observed a few more bands than (1) as well as Cl isotope shifts. The lower-state constants for these two systems agree poorly with those derived from the $b \rightarrow X$ bands (6).

^dP and Q heads.

^eSingle sequence of P heads.

^fFrom the P heads of the $b \rightarrow X$ transitions.

(1) Ferguson, Hudes, PR 57, 705 (1940).

(2) Basco, Yee, SpL 1, 19 (1968).

(3) Avasthi, SpL 3, 291 (1970).

(4) Danon, Chatalic, Pannetier, CR C 272, 1411 (1971).

(5) Briggs, Kemp, JCS FT II 68, 1083 (1972).

(6) de Bie-Prévot, Thèse (U. Libre de Bruxelles, 1974).

SbF: ^a Ω -type doubling $\Delta v_{ef}(v=0) = (+)8.9 \times 10^{-5} J(J+1)$. The rotational analyses by (4) and (5) are in disagreement with (8).

^bExtrapolations from $v'-0$ bands having $v' \geq 2$.

^cExtrapolations from $v'-0$ ($A_2 \rightarrow X_2$) and $0-v''$ ($A_2 \rightarrow a$) bands having $v' \geq 1$ and $v'' \geq 2$, respectively.

^dExtrapolated from the 0-2 band, the only rotationally analysed band. The lower-state vibrational numbering of (6) has been increased by 1 (9).

^eBand heads observed, but no details given (9).

^f Ω -type doubling $\Delta v_{ef}(v=0) = +0.00031 J(J+1)$ (9).

(1) Rochester, PR 51, 486 (1937).

(1a) Howell, Rochester, PPS 51, 329 (1939).

(2) Patel, Abraham, IJPAP 7, 641 (1969).

(3) Abraham, Patel, JP B 3, 882 (1970).

(4) Abraham, Patel, JP B 3, 1183 (1970).

(5) Abraham, Patel, JP B 4, 1398 (1971).

(6) Chakravorty, Abraham, Patel, JP B 6, 757 (1973).

(7) Wang, Jones, Prévot, Colin, JMS 49, 377 (1974).

(8) Prévot, Colin, Jones, JMS 56, 432 (1975).

(9) Vasudev, Jones, JMS 59, 442 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(I21)Sb ¹ H		($\mu = 0.99949368$)								JUL 1977
$A_3(^3\Pi) 0^+$	[30115.8]			[4.10]			[2.02 ₈]	$A_3 \leftarrow X_2, R$	29460.8 Z	(1)(2)
B	0^+ [29761.2]			[4.06]			[2.03 ₈]	$A_3 \leftarrow X_1, R$	30115.8 Z	
$A_2(^3\Pi) 1$	[28541]	Very diffuse bands, rotational structure not resolved.						$B \leftarrow X_2, R$	29106.2 Z	
$A_1(^3\Pi) 2$	[26901]							$B \leftarrow X_1, R$	29761.2 Z	
$X_2(^3\Sigma^-) 1$	[654.97]							$A_2 \leftarrow X_2, R$	27886 H	
$X_1 0^+$	[0]							$A_1 \leftarrow X_2, R$	26246 H	
				[5.684] ^a		[2.4]	[1.722 ₆]			
(I21)Sb ² H		($\mu = 1.98109965$)								JUL 1977
C	0^+ [30566.4]			[1.95]			[2.09]	$C \leftarrow X_2, R$	29906.4 Z	(1)
$A_3(^3\Pi) 0^+$	[30159.5]			[2.06]			[2.03]	$A_3 \leftarrow X_2, R$	29499.5 Z	
B	0^+ [29959.8]			[2.10]			[2.01]	$A_3 \leftarrow X_1, R$	30159.5 Z	
$A_2(^3\Pi) 1$	[28677]	Diffuse, partly resolved rotational structure. Fragments only.						$B \leftarrow X_2, R$	29299.8 Z	
$A_1(^3\Pi) 2$	[27017.9]							$B \leftarrow X_1, R$	29959.8 Z	
$X_2(^3\Sigma^-) 1$	[660.01]							$A_2 \leftarrow X_2, R$	28017.3 H	
$X_1 0^+$	[0]							$A_1 \leftarrow X_2, R$	26357.9 Z	
				[2.53]		[10]	[1.83]			
				[2.8782] ^b		[0.45]	[1.7194]			
(I21)Sb ¹²⁷ I		($\mu = 61.915748_2$)								JUL 1977
C ($^3\Pi$)	(41909)	[264]	H					C ← X, V	41942 H	(1)
	(41387)	[247]	H						41411 H	
	(40846)	[244]	H						40869 H	
X	0	[198]	H							

State	T _e	ω _e	ω _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
								Design.	v ₀₀		
(121)Sb ¹⁴ N		(μ = 12.5495824 ₂)								JUL 1977 A	
B (1Π)	34465	830.7	H	6.0				B↔X, R	34409	H	(1)* (2)
X 1Σ ⁺	0	942.0	H	5.6							
(121)Sb ¹⁶ O		(μ = 14.1261081 ₁) D ₀ ⁰ ≤ 4.39 eV (see ^c)								JUL 1977	
E 2Σ ⁽⁺⁾	39785	849.4 ^a	H ^Q	2.9				E↔X, V	37531 39802	H ^Q	(2)(5)
F (2Δ)	(38958)	[588.5]	H ^Q					F↔X, R	36573.7 38844.5	H ^Q	(5)
G		Diffuse heads 35800 - 38950 cm ⁻¹ .						G↔X, (V)			(5)
D 2Π _½	34544	505.9 ^b	H	3.0	B ₁ = 0.2777 ^c	D ₁ = 4.0	r ₁ = 2.073	D→X ^d , R	34389.5 ^e		(3)*(5)*(7)*
C (2Δ _r)	30315 29747	568.1 570.6	H	3.28 3.52	B ₂ = 0.2991 ^f	D ₂ = 3.25	r ₂ = 1.997	C→X, R	27919.6 29624.8 ^g	H	(3)*(5)*(8)*
B 2Σ	26594	582.0	H ^Q	6.5				B→X, R	24204 26476	H ^Q	(1)(3)* (4)*
A 2Π _r	20801 20668	569.0	H	5.0				A→X, R	18405 20544	H	(1)
X 2Π _r	2272 0	816	H ^Q	4.2	0.3580 ^{fh}	0.0022	[2.7]				

Sb¹H, Sb²H:

^aSpin splitting constants $\lambda = +333.39$, $\gamma = -0.44$.

^bSpin splitting constants $\lambda = +333.01$ (slight J dependence), $\gamma = -0.19$.

(1) Bollmark, Lindgren, CPL 1, 480 (1967); PS 10, 325

(2) Basco, Yee, SpL 1, 13 (1968). | (1974).

SbI: (1) Danon, Chatalic, Deschamps, Pannetier, CR C 269, 1249 (1969).

SbN: (1) Coy, Sponer, PR 58, 709 (1940).

(2) Ciach, Thistlethwaite, JCP 53, 3381 (1970).

SbO: ^aFrom the analysis by (5).

^bVibrational numbering of (5) increased by 1; see (6)(7).

^c $v=2$ of D $^2\Pi_{\frac{1}{2}}$ predissociated at low J.

^dX $^2\Pi_{\frac{1}{2}}$ component.

^eCalculated from the origin of the 1-1 band.

^fRotational constants for ¹²¹SbO.

(continued p. 575)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{121}\text{Sb}^{31}\text{P}$		$\mu = 24.6570049$ $D_0^0 = 3.68 \text{ eV}^a$								JUL 1977
B $^1\Pi$	28136	[394.0] ^b	Z	0.127 ₇ ^b	0.000 ₂	(3)	2.31 ₄	B → X, R	28083.69 Z	(1)* (3)*
X $^1\Sigma^+$	0	500.07	Z	1.632 ^c	0.1406	0.0005	0.4			
$(^{121})\text{Sb}^{32}\text{S}$		$(\mu = 25.2855155)$								JUL 1977
		Additional unassigned emission bands (both V and R shaded) in the region 12000 - 28500 cm^{-1} .								(1)
G		(380)	H	(4.4)				G → (X), R	24626.0 H 27026.6 H	(1)
F		(296)	H					F ↔ X, R	27406.0 H 28664.0 H	(1)*
E		(442)	H					E ↔ X, R	26248.3 H 26720.4 H	(1)*
D		(389)	H					D ↔ X, R	24310.4 H	(1)*
C		(390)	H					C → X, R	23249.3 H 25996.4 H	(1)*
B		(397)	H	(16.5)				B → (X), R	22517.2 H	(1)*
A		(341)	H					A ↔ X, R	19472.6 H 22278.9 H	(1)*
X $^2\Pi_r$		(470) (480)	H H	(1.6) (1.2)						
$(^{121})\text{Sb}^{(80)}\text{Se}$		$(\mu = 48.113717_0)$								JUL 1977
D	43756	365.7 ₄	H	0.76				D ← X, V	43776 H	(1)
C	(41600)	Unassigned V shaded bands 40700 - 42500 cm^{-1} .						C ← X, V		(1)
B	36041	418.0	H	0.48				B ← X, V	36087 H	(1)
A	28965	221.8	H	1.0				A ← X, R	28913 H	(1)
X	0	326.1	H	1.04						

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
$(^{121}\text{Sb } ^{130}\text{Te})$		$(\mu = 62.621731_g) \quad D_0^0 = 2.8 \text{ eV}^a$								JUL 1977
A	43553	314.5	H	0.48				A ← X,	V 43568	H (1)
X	0	284.4	H	0.20						

SbO (continued):

^eCalculated from the origin of the 2-0 band (^{121}SbO).

^h Λ -type doubling in $^2\Pi_{3/2}$; $\Delta v = 0.107(J+\frac{1}{2})$.

- (1) Sen Gupta, IJP 13, 145 (1939).
- (2) Sen Gupta, IJP 17, 216 (1943).
- (3) Lakshman, ZP 158, 367 (1960).
- (4) Lakshman, ZP 158, 386 (1960).
- (5) Shimauchi, SL 2, 109 (1960).
- (6) Rao, Rao, CS 37, 310 (1968).
- (7) Rai, Upadhyaya, Rai, JP B 3, 1374 (1970).
- (8) Rai, Rai, Rai, CJP 52, 592 (1974).

SbP: ^aThermochemical value (mass-spectrom.) (2).

^b $\Delta G(3/2) = 395.6$; strong perturbations in $v=0$ and 1 make the evaluation of equilibrium constants not very meaningful.

^c $\omega_e y_e = +0.0025$.

- (1) Yee, Jones, Kopp, JMS 33, 119 (1970).
- (2) Kordis, Gingerich, JPC 76, 2336 (1972); JCP 58, 5141 (1973).
- (3) Jones, Flinn, Yee, JMS 52, 344 (1974).

SbS: (1) Shimauchi, Nishiyama, SL 17, 76 (1968).

SbSe, SbTe:

^aThermochemical value (mass-spectrom.) (2), recalculated with the revised value for the dissociation energy of Te_2 .

- (1) Sharma, PPS A 66, 1109 (1953).
- (2) Porter, Spencer, JCP 32, 943 (1960).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{45}\text{Sc}_2$		$\mu = 22.477958_7$ $D_0^0 = 1.6_5 \text{ eV}^a$								MAY 1975
$^{45}\text{Sc}^{35}\text{Cl}$		$\mu = 19.6692074$ $D_0^0 = (3.4) \text{ eV}$								MAY 1975
y	x + 27189.7	482.7	H^Q	2.5				y \rightarrow x, ^a	V 27202.0	H^Q (2)
x	x	458.2	H^Q	2.8						
e ($^3\Pi$)	d + 22260.0	312.5	H^Q	0.55				e \rightarrow d, V	22461.0 H_P^P 22361.5 H_P^P 22267.6 ^b H^Q	(1)(2)
d ($^3\Sigma$)	d	297.3	H^Q	0.61						
c ($^3\Delta$)	a + 13113.8	355.9	H	2.18				c \rightarrow a, R	13096.1 H 13092.4 H 13090.7 H	(1)(2)
b ($^3\Phi$)								b \rightarrow a, R	12596.2 H 12567.6 H 12537.6 H	(1)(2)
a ($^3\Delta$)	a	398.3	H	1.36						
F ($^1\Pi$)	31249.9	364.7	H	1.0				F \rightarrow X, R	31208.8 H	(1)(2)
E ($^1\Sigma^+$)	27033.3	472.1	H	1.32				E \rightarrow X, R	27045.8 H	(1)(2)
D ($^1\Pi$)	21521.1	373.1	H^R	1.6	[0.1569] ^c	[1.6]	[2.337]	D \rightarrow X, R	21484.0 H^R	(1)(2)
B ($^1\Pi$)	17613.3	374.3	H^R	2.3	[0.1551] ^c	[1.1]	[2.351]	B \rightarrow X, R	17576.6 H^R	(1)(2)
A ($^1\Sigma^+$)	12431.2	373.9	H	0.9	[0.1574]	[1.1]	[2.333]	A \rightarrow X, R	12394.7 H	(1)(2)
X ($^1\Sigma^+$)	0	447.4	H	1.8	0.1725	0.0010	[1.1]		2.229	

Sc₂: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1) Verhaegen, Smoes, Drowart, JCP 40, 239 (1964).
- (2) Verhaegen, PhD Thesis, University of Brussels (1965)
[quoted by Drowart in "Phase Stability in Metals and Alloys"; Rudman, Stringer, Jaffee, Eds.; McGraw-Hill (1967)].

ScCl: ^aUnidentified system.

^bP head at 22263.1 cm⁻¹.

^cSmall Λ -type doubling.

- (1) Shenyavskaya, Mal'tsev, Gurvich, VMUK 22(4), 104 (1967)
- (2) Shenyavskaya, Mal'tsev, Kataev, Gurvich,
OS(Engl. Transl.) 26, 509 (1969).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (Å)	Observed Transitions		References	
								Design.	v_{00}		
$^{45}\text{Sc}^{19}\text{F}$										MAY 1975	
H 1Π		$\mu = 13.3546988$		$D_0^0 = 6.17 \text{ eV}^a$							
				[0.3671] ^b			[1.854 ₃]	H ↔ X, R	38806.1 Z	(5)(9)	
		0-0 sequence of V shaded absorption bands. Complex structure.									(5)(9)
G 1Π	35009	[570] H		[0.378] ^{bc}			[1.82 ₇]	G ↔ X, R	34926.7 ^d Z	(1)(2)(5)	
				[0.346 ₃]			[1.909 ₂]		27202.2 Z		
G $3\phi_4$				[0.344 ₁]			[1.915 ₃]	g ← a, R	27171.1 Z	(5)	
G $3\phi_3$				[0.341 ₃]			[1.923 ₁]		27138.2 Z		
F 1Π	26891.5	[565.3] Z (3.1)		0.3461 ^e	0.0025		1.909 ₈	F ← X, R	26809.6 Z	(2)(5)	
		Complex group of R shaded absorption bands.									(5)
		Strong 0-0 sequence of V shaded bands. ^f									(5)(7)(9)
E 1Π	20383.5	622.1 Z 3.7		0.3630 ^{bc}	0.00296		1.864 ₈	E ↔ X, R	20326.8 Z	(2)(4)(5)(7)	
				[0.3677] ^b			[1.852 ₈]		18361.4 Z		
d ($3\Pi_2$)								d ← a, R	18336.0	(5)	
d ($3\Pi_1$)											
C $1\Sigma^+$	16164.7	589.6 Z 2.64		0.3473	0.0024		1.906 ₅	C ↔ X, R	16092.0 Z	(2)(4)(5)	
				0.3545	0.00310		1.887 ₀		15317.6 Z		
c $3\phi_4$ g	$a_3 + 15356.9$			[0.3511]			[1.896 ₁]	c ↔ a, R	15277.5 Z	(3)(5)(7)	
c $3\phi_3$ g	$a_2 + 15316.8$	570.4 Z 2.96		[0.3490]			[1.901 ₈]		15234.4 Z		
c $3\phi_2$ g	$a_1 + 15273.6$										
B 1Π g	10735.4 ₉	586.25 Z 2.015 ^h		0.3431 ₀ ⁱ	0.0026 ₂ ^j		1.9181	B ↔ X, R	10661.25 Z	(4)(5)(10)	
a $3\Delta_3$ g	a_3 k	649.1 ₁ Z		0.3706	0.00258		1.845 ₆				
a $3\Delta_2$ g	a_2 k	648.9 ₈ Z	3.03	0.3665	0.00254		1.855 ₉				
a $3\Delta_1$ g	a_1 k	648.9 ₁ Z		0.3623	0.00250		1.866 ₆				
X $1\Sigma^+$	0 ^l	735.6 Z 3.8		0.3950	0.00266		1.787 ₇				

ScF: ^aThermochemical value (mass-spectrom.)(8).
^bPerturbations.
^cB values are for the f levels.
^dFrom (2); 34920.7 in (5) appears to be a misprint.
^e Λ -type doubling $\Delta v_{fe} = + 0.0021 \times J(J+1)$.
^fThe authors of (5) assume the bands to arise from a transition ${}^3\Delta \leftarrow {}^3\Delta$ with nearly equal coupling constants in both states. The upper state, then, has $\omega_e = 724.7$, $\omega_e x_e = 3.64$. The system was also observed in emission by (7) who interpreted it as ${}^3\Pi \rightarrow {}^3\Sigma$ with $\omega'_e = 591.0$, $\omega'_e x'_e = 2.73$, $\omega''_e = 514.1$, $\omega''_e x''_e = 1.98$. Neither (5) nor (7) give enough details.
^gFor a reassignment of molecular orbital configurations see (11).
^h $\omega_e y_e = - 0.0633$.
ⁱ Λ -type doubling $\Delta v_{fe} \begin{cases} (v=0) = + 1.115 \\ (v=1) = + 0.714 \\ (v=2) = + 0.452 \\ (v=3) = + 0.315 \end{cases} \times 10^{-3} J(J+1) - \dots$
^j $\gamma_e = + 3.25 \times 10^{-5}$.
^kTheoretical calculations by (6) put the a ${}^3\Delta$ state at 461 cm^{-1} and the corresponding ${}^1\Delta$ state at 2612 cm^{-1} above X ${}^1\Sigma^+$.
^lThat X ${}^1\Sigma^+$ is the ground state is strongly suggested by the fact that only B \leftarrow X, C \leftarrow X, and E \leftarrow X, but none of the triplet systems, were observed in matrix absorption at 4 K (4).

ScF (continued):

- (1) Gurvich, Shenyavskaya, OS(Engl. Transl.) 14, 161 (1963).
- (2) Barrow, Gissane, Le Bargy, Rose, Ross, PPS 83, 889 (1964).
- (3) Barrow, Gissane, PPS 84, 615 (1964).
- (4) McLeod, Weltner, JPC 70, 3293 (1966).
- (5) Barrow, Bastin, Moore, Pott, Nature 215, 1072 (1967).
- (6) Carlson, Moser, JCP 46, 35 (1967).
- (7) See ref. (1) of ScCl.
- (8) Zmbov, Margrave, JCP 47, 3122 (1967).
- (9) Barrow, in DONNSPEC (1970).
- (10) Barrow, Pedersen, JP B 4, L11 (1971).
- (11) Scott, Richards, CPL 28, 101 (1974).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{45}\text{Sc}^1\text{H}$ $^{45}\text{Sc}^2\text{H}$		$\mu = 0.98572711$ $\mu = 1.92773633$ Weak emission bands in the green ($\sim 17900\text{ cm}^{-1}$) and near infrared ($11800 - 12300\text{ cm}^{-1}$); absorption bands of complex structure in the region $17690 - 18350\text{ cm}^{-1}$; no analysis. Theoretical calculations (2)(3) predict a $^1\Sigma^+$ or $^3\Delta$ ground state, and a dissociation energy of $\sim 1.8\text{ eV}$.								OCT 1977 (4)* (1)*
$^{32}\text{S}(^{35})\text{Cl}$		$(\mu = 16.7016919_7)$ A single progression of absorption bands starting at 22644 cm^{-1} with a spacing of $460 - 490\text{ cm}^{-1}$ and tentatively assigned to SCl has been observed in the flash photolysis of S_2Cl_2 (1).								JUL 1977
$^{45}\text{Sc}^{16}\text{O}$		$\mu = 11.7974775_7$ $D_0^0 = 6.96\text{ eV}^a$								JAN 1977 A
B $^2\Sigma^+$ 20645.1		825.4 ₇ Z 4.2 ₁	[0.48308] ^{bc}	0.0032	[6.74]	[1.7198 ₆]	$B \leftrightarrow X, ^d \text{R}$ 20571.15 Z			(1)(2)(3)(4)* (5)*(6)*(7)* (8)(14)(15)*
A $^2\Pi_r$ 16547.0 ^e		876.0 ^f H 5.0 ₀	[0.50277] ^g	(0.0037)	[6.5 ₄]	[1.6858 ₅]	$A \leftrightarrow X, ^d \text{R}$ 16498.13 ^h Z			(1)(2)*(3) (4)*(5)*(6)* (7)*(8)(14) (16)(18)*
A' $^2\Delta_r$ 15135.9 ⁱ X $^2\Sigma^+ k$ 15029.8 0		845.9 H 4.9 [964.9 ₅] Z 4.2 ₀ H	[0.51343] ^{lc}	0.0033	[5.85]	[1.6682 ₆]	$A' \rightarrow X, ^j \text{R}$ 15072.0 ^j 14965.9 ^j H ESR sp. ^m			(21)
$^{45}\text{Sc}^{32}\text{S}$		$\mu = 18.6841468$ $D_0^0 = 4.9_2\text{ eV}^a$								JAN 1977
B $^2\Sigma$ 12497.6		488.2 H 2.0					$B \rightarrow X, \text{R}$ 12459.0 H			(4)
A $^2\Pi$		Emission bands in the region $11000 - 12600\text{ cm}^{-1}$, v' numbering unknown. Progression of absorption bands in Ne matrix, $11100 - 12500\text{ cm}^{-1}$, tentatively attributed to ScS (2).					$A \rightarrow X, \text{R}$ (11150) (11040)		(4)	
X $^2\Sigma$ 0		565.2 ^b H 1.8					ESR sp. ^c			

Sc¹H, Sc²H:

- (1) Smith, PRS A 332, 113 (1973).
- (2) Scott, Richards, JP B 7, 1679 (1974).
- (3) Kunz, Guse, Blint, JP B 8, L358 (1975).
- (4) Bernard, Effantin, Bacis, CJP 55, 1654 (1977).

ScI: (1) Donovan, Husain, Jackson, TFS 64, 1798 (1968).

ScO: ^aThermochemical value (mass-spectrom.)(11)(12)(13).

^bSpin-splitting constant $\gamma_0 = (-)0.0670$.

^cPotential energy curves (20).

^dIntensity distribution (19)(22).

^e $A_0 = +115.33$; slight J dependence.

^fCorrected for head-origin separations.

^g Λ -type doubling in $^2\Pi_{1/2}$, $\Delta v_{fe}(v=0) = -0.0655(J+\frac{1}{2}) + \dots$, and in $^2\Pi_{3/2}$ [see (18)].

^h $J'=\frac{1}{2}$ (average of F_1 and $\{F_2\}$) relative to $N''=0$. The sub-band origins ($\{J'=0\}$ relative to $N''=0$) are at 16440.61 and 16554.83 cm^{-1} .

ⁱ T_e in good agreement with theoretical predictions (9) (21).

^jObserved in the "single-collision" Sc + O₂ chemiluminescence spectrum.

^kThe $^2\Sigma$ character of the ground state was theoretically predicted by (9) and experimentally verified by (10)(14) [ESR spectrum and matrix absorption].

^lLarge magnetic hyperfine structure, $4b = +0.254$ (15)(18) [see also (10)(14)].

^mIn rare gas matrices (10)(14)(17).

(1) Johnson, Johnson, PRS A 133, 207 (1931).

(2) Meggers, Wheeler, JRNBS 6, 239 (1931).

(3) Jevons, "Band Spectra of Diatomic Molecules", Phys. Soc. London (1932).

ScO (continued):

(4) Piccardi, GCI 63, 127 (1933).

(5) Gatterer, RS 1, 153 (1942).

(6) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(7) Åkerlind, AF 22, 41 (1962).

(8) Ortenberg, Glasko, Dimitriev, SAAJ 8, 258 (1964).

(9) Carlson, Ludeña, Moser, JCP 43, 2408 (1965).

(10) Kasai, Weltner, JCP 43, 2553 (1965).

(11) Ames, Walsh, White, JPC 71, 2707 (1967).

(12) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).

(13) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).

(14) Weltner, McLeod, Kasai, JCP 46, 3172 (1967).

(15) Adams, Klemperer, Dunn, CJP 46, 2213 (1968).

(16) Athénour, Bacis, Féménias, Stringat, CR B 271, 567

(17) McIntyre, Lin, Weltner, JCP 56, 5576 (1972). | (1970).

(18) Stringat, Athénour, Féménias, CJP 50, 395 (1972).

(19) Féménias, Athénour, Stringat, CJP 52, 361 (1974); 53, 2353 (1975) (erratum).

(20) Narasimhamurthy, Murthy, Pramāṇa 2, 269 (1974).

(21) Chalek, Gole, JCP 65, 2845 (1976).

(22) Féménias, Goure, Stringat, CJP 55, 180 (1977).

ScS: ^aThermochemical value (mass-spectrom.)(1); (3) give a slightly lower value.

^bIR spectrum in Ar matrix at 4 K gives $\Delta G(\frac{1}{2}) = 554$ (2).

^cIn Ar matrix at 4 K (2).

(1) See ref. (12) of ScO.

(2) See ref. (17) of ScO.

(3) Tuenge, Laabs, Franzen, JCP 65, 2400 (1976).

(4) Stringat, Fenot, CJP 54, 2293 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$4^5\text{Sc}(^{80})\text{Se}$		$(\mu = 28.771125_4)$ $D_0^0 = 3.9_6 \text{ eV}^a$							MAY 1975	
$4^5\text{Sc}(^{130})\text{Te}$		$(\mu = 33.398044_4)$ $D_0^0 = 3.0_5 \text{ eV}^a$							MAY 1975	
$^{80}\text{Se}_2$		$\mu = 39.958262_7$ D_0^0 , see ^a . I.P. = 8.88 eV^b							JUL 1977	
F	(1_u) (55421)	[430.2]	H					$(F \leftarrow X_2)$ V	54932.8 H	(13)
E	0_u^+ 54752.5	403.9	H 1.3	0.0924	0.00033		2.13_7	$E \leftarrow X_2$, ^c V	54249	(13)(22)
								$E \leftarrow X_1$, V	54761.7 H	(13)
D	(1_u) (53075)	[426.2]	H	[0.0965]			[2.09 ₁]	$D \leftarrow X_1$, ^d V	53096.1 H	(13)*
C ₂	$3\Sigma_u^- 0_u^+$ (53324)	[414]	H	Diffuse bands				$C_2 \leftarrow X_1$, V	53339 H	(13)
C ₁	1_u 53220.5	428.0	H 1.22	0.09664	0.00033 ₃		2.089_4	$C_1 \leftarrow X_2$, V	52730.9 Z	(13)*
B ₂	1_u 26058.6	246.42 ^e	Z 1.225	0.07086 ^{fg}	0.00055 ₃	(2)	2.440_0	$B_2^h \leftrightarrow X_2^i$, R	25478.2 ^j	(5)
	$3\Sigma_u^-$							$B_2 \rightarrow X_1$, R	25989.2	(21)(22)
B ₁	0_u^+ 25980.36	246.291 ^{ek}	Z 1.016 ^l	0.07048 ^m	0.000345	(4)	2.446_6	$B_1 \rightarrow X_2$, R	25399.8	(21)(22)
								$B_1 \leftrightarrow X_1^i$, R	25910.84 Z	(5)*
X ₂	1_g 510.0 ⁿ	387.156 ^o	Z 0.9640 ^o	0.09019 ^{op}	0.000299 ^o	(2)	2.162_8			
X ₁	$3\Sigma_g^- 0_g^+$ 0	385.303	Z 0.9636 ₃ ^q	0.08992	0.000288 ^r	2.4^s	2.166_0	t		

ScSe: ^aThermochemical value (mass-spectrom.)(1)(2).

- (1) Bergman, Coppens, Drowart, Smoes, TFS 66, 800
 (2) Ni, Wahlbeck, HTS 4, 326 (1972). (1970).

ScTe: ^aThermochemical value [(1), no details].

- (1) See ref. (1) of ScSe.

Se₂: ^aFrom the predissociation in $B_1 0_u^+$ (see ^m) three possible spectroscopic values for the dissociation energy of $^{80}\text{Se}_2$, i.e. $D_0^0 = 3.410_5$, 3.163_8 , 3.096_4 eV , can be derived depending on the assumed atomic states at the observed predissociation limits. (5) prefer $D_0^0 = 3.164 \text{ eV}$ on the basis of indirect spectroscopic arguments. However, both photoionization (10)(24) and thermochemical studies [mass-spec-

Se₂ (continued):

trometry (6)(9)(12), Knudsen-torsion effusion (8); see also (11)(17)] strongly favour the higher value $D_0^0 = 3.411$ eV.

^bPhotoionization mass-spectrometry (10). From the photo-electron spectrum (23) derive adiabatic and vertical ionization potentials of 8.70 and 8.89 eV, respectively.

^cThis transition is much weaker than $E \leftarrow X_1$.

^dThe assumption (13) that this transition is $C_1 \leftarrow X_1$ has been withdrawn (22) since it gives the wrong $X_1 - X_2$ splitting.

^eVibrational analysis confirmed by isotope investigations

^fAverage value, $B_e(F_3) - B_e(F_2) = +0.00038$. | (5).

^gRotational perturbations; a tentative analysis (18) of these and similar perturbations in the O_u^+ component was based on an erroneous value of the $O_u^+ - l_u$ splitting. Predissociation in $v=5$ at $J=72(F_3)$ and $73(F_2)$; bands with $v'=6$ have not been seen.

^hLifetime $\tau(v=0, J=105) = 58$ ns, from Hanle effect measurements (19)(20) combined with experimentally determined Landé g_J factors (20)(25).

ⁱVarious proposed other "systems" in the region 14500 - 18500 cm⁻¹ (1)(4) have been shown (5) to belong to the main B-X system. (18) have extended the rotational analysis of the ⁷⁸Se₂ bands to higher values of v'' .

^jExtrapolated from bands having $v'' \geq 8$, using lower state constants of (14).

^kThe $B_1 O_u^+$ state has a substantial potential maximum arising from an avoided crossing with a repulsive O_u^+ state. The interaction strongly affects vibrational levels above $v=15$; the theoretical discussion by (16) predicts irregular level shifts and widths above the crossing point.

^l $w_e y_e = -0.00549$.

^mSharp predissociation limits occur for $v=4(J=106)$, $v=5(J=82)$, $v=6(J=50)$, leading to a dissociation limit at 27508 cm⁻¹ above $X_1 O_g^+(v=0)$, and for $v=13(J=96)$, $v=14(J=78)$, $v=15(J=50)$, leading to a dissociation limit at 29498 cm⁻¹. (5) attribute the former to $^3P_2 + ^3P_1$, the latter to $^3P_1 + ^3P_1$. There are many rotational perturbations and several accidental predissociations; see also ^g.

ⁿFrom (22) whose measurements of fluorescence series in the range $6 \leq v'' \leq 12$ lead to $\Delta v = +509.95 + 2.1256(v + \frac{1}{2})$ for the separation of the rotationless l_g and o_g^+ substates.

^oConstants apply to $8 \leq v \leq 29$.

^pAverage of F_2 and F_3 , $B_e(F_3) - B_e(F_2) = +0.00006$.

^q $w_e y_e = -0.0008184$.

^r $r_e = -6.1 \times 10^{-7}$.

^s $\beta_e = -0.023 \times 10^{-8}$.

^tFor a theoretical calculation of the magnetic moment of Se₂, consistent with experimental results, see (20a).

- (1) Rosen, Monfort, Physica 3, 257 (1936).
- (2) Shin-Piaw, AP(Paris) (11) 10, 173 (1938).
- (3) Migeotte, BSRSL 10 (12), 658 (1941).
- (4) Leelavathi, Rao, IJP 29, 1 (1955).
- (5) Barrow, Chandler, Meyer, PTRSL A 260, 395 (1966).
- (6) Berkowitz, Chupka, JCP 45, 4289 (1966).
- (7) Drowart, Goldfinger, QR 20, 545 (1966).
- (8) Budininkas, Edwards, Wahlbeck, JCP 48, 2867 (1968).
- (9) Colin, Drowart, TFS 64, 2611 (1968).
- (10) Berkowitz, Chupka, JCP 50, 4245 (1969).
- (11) Meschi, Searcy, JCP 51, 5134 (1969).
- (12) Uy, Drowart, TFS 65, 3221 (1969).

(continued p. 585)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(^{80}\text{Se})\text{Se}_2^+$		$(\mu = 39.958125_5) \quad D_0^0 = 4.3_8 \text{ eV}^a$							JUL 1977	
D ($^2\Pi_u$)	41210	From the maxima of the observed photoelectron peaks (2); vibrational structure unresolved. Additional partly resolved peaks in the region 17.3-20.6 eV above $X \ ^3\Sigma_g^-$ of Se_2 (2).								
C ($^2\Sigma_g^-$)	35650									
B ($^2\Pi_u$)	(31620)									
b ($^4\Sigma_g^-$)	27260									
A ($^2\Pi_u$)	19200									
a ($^4\Pi_u$)	14440									
X ₂ ($^2\Pi_{g\frac{3}{2}}$)	1940									
X ₁ ($^2\Pi_{g\frac{1}{2}}$)	0									
$^{80}\text{Se}_2^-$		$\mu = 39.958399_8$							JUL 1977	
A ($^2\Pi_u$)	(16173)	216.7	0.61 ₅	Constants for Se_2^- ions dissolved in KI crystals, from fluorescence and absorption spectra studied at 2 K (4)(5).				A \leftrightarrow X,	16192 ^a 16040	(2)(4)(5)
X ($^2\Pi_g$)	0	330.3	0.86					Raman sp. ^b EPR sp. ^b		(3) (1)
$(^{80}\text{Se})^{(79)}\text{Br}$		$(\mu = 39.707146_1)$							JUL 1977	
B ₂ ($^2\Pi$)	(x + 46158)	[390]	H					B ₂ \leftarrow X ₂ , ^a v	46195	H (1)
B ₁ ($^2\Pi$)	47227.3	392.5	H	2.0				B ₁ \leftarrow X ₁ , ^a v	47265	H (1)
X ₂ ($^2\Pi_1$)	x									
X ₁ ($^2\Pi_1$)	0	316.9	H	0.7						
$(^{80}\text{Se})^{(35)}\text{Cl}$		$(\mu = 24.3250212)$							JUL 1977	
A ($^2\Pi_1$)		[595]	H	Single progression consisting of seven bands ^b ; vibrational numbering uncertain.				A \leftarrow X, ^a R	27116	H (1)
X ($^2\Pi_1$)	0									

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(⁸⁰)Se ¹⁹ F X $2\Pi_i$ 0^b		($\mu = 15.3494168$) (757) ^a		$D_0^0 = (3.2_1) \text{ eV}^a$ [0.3624]			[1.7408]	ESR sp. ^c		JUL 1977 (1)(3)

Se₂ (continued):

- (13) Barrow, Burton, Callomon, TFS 66, 2685 (1970).
- (14) Barrow, Beattie, Burton, Gilson, TFS 67, 583
- (15) Tatum, Watson, CJP 49, 2693 (1971). | (1971).
- (16) Atabek, Lefebvre, CPL 17, 167 (1972).
- (17) Smoes, Mandy, Auwera-Mahieu, Drowart, BSCB 81,
45 (1972).
- (18) Yee, Barrow, JCS FT II 68, 1181 (1972).
- (19) Dalby, Vigué, Lehmann, CJP 53, 140 (1975).
- (20) Gouedard, Lehmann, CR B 280, 471 (1975).
- (20a) Büchler, Meschi, JCP 63, 3586 (1975).
- (21) Gouedard, Lehmann, JP B 9, 2113 (1976).
- (22) Greenwood, Barrow, JP B 9, 2123 (1976).
- (23) Streets, Berkowitz, JESRP 9, 269 (1976).
- (24) Radler, Berkowitz, JCP 66, 2176 (1977).
- (25) Gouedard, Lehmann, JP(Paris) 38, L-85 (1977).

Se₂⁺: ^aValue obtained by photoionization mass-spectrometry
(1), consistent with the highest of three possible
spectroscopic values for $D_0^0(\text{Se}_2)$ [see ^a of Se₂].
(1) See ref. (10) of Se₂.
(2) See ref. (23) of Se₂.

SeF (cont'd): (3) Brown, Byfleet, Howard, Russell, MP 23, 457 (1972).
(4) O'Hare, JCP 60, 4084 (1974).

Se₂⁻: ^aSplitting due to the crystal field, not spin-orbit coup-
^bIn NaI and KI crystals. | ling.

- (1) Vannotti, Morton, JCP 47, 4210 (1967).
- (2) Rolfe, JCP 49, 4193 (1968).
- (3) Holzer, Murphy, Bernstein, JMS 32, 13 (1969).
- (4) Ikezawa, Rolfe, JCP 58, 2024 (1973).
- (5) Vella, Rolfe, JCP 61, 41 (1974).

SeBr: ^aObserved in the flash photolysis of Se₂Br₂.

- (1) Oldershaw, Robinson, TFS 67, 907 (1971).

SeCl: ^aObserved in the flash photolysis of SeCl₂. The assignment
of this spectrum to SeCl is not certain; it is assumed
that only one component of $2\Pi-2\Pi$ is observed because of
large doublet splitting in the lower state.

^bThe first and last bands of the progression are diffuse.

- (1) Ciach, Power, Thistlethwaite, CPL 9, 349 (1971).

SeF: ^aTheoretical estimate (4).

^b A_0 (observed) \approx -560 (1), A_0 (calculated) = -1790 (3).

^c $\mu_{el} = 1.52 \text{ D}$ (2). Magnetic hfs parameter, rotational and
third-order g factors (3).

- (1) Carrington, Currie, Miller, Levy, JCP 50, 2726 (1969).
- (2) Byfleet, Carrington, Russell, MP 20, 271 (1971).



State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
($^{80}\text{Se}^1\text{H}$)										
F		$(\mu = 0.99527385)$		$D_0^0 = (3.2) \text{ eV}^a$		$\text{I.P.} = (9.8) \text{ eV}^b$		$F \leftarrow X_1$, 71190		(5)
E				Weak diffuse band.				$E \leftarrow X_1$, 69604		(5)
D				Diffuse band.				$D \leftarrow X_1$, 66814		(5)
C				Strong diffuse band.				$C \leftarrow X_1$, R 55797	H^Q	(5)
A ($^2\Sigma^+$)	(31500)	[1232] (H) (172) ^c		Strong double-headed band.				$A \leftarrow X_1$, R 31048	(H)	(2)
X_2 $^2\Pi_{1/2}$	(1815) ^d			Diffuse bands.						
X_1 $^2\Pi_{3/2}$	0	(2400) ^c		[7.78] ^e			[1.47 ₅]	ESR sp. ^f		(1)(3)(4)
($^{80}\text{Se}^2\text{H}$)										
A ($^2\Sigma^+$)	(31490)	$(\mu = 1.96458951)$		$D_0^0 = (3.2) \text{ eV}^a$				$A \leftarrow X_1$, R 31178	(H)	(2)
X_2 $^2\Pi_{1/2}$	(1815) ^d	[959] (H) (87) ^c		Diffuse bands.						
X_1 $^2\Pi_{3/2}$	0	(1708) ^c		[3.94 ₀] ^e			[1.47 ₆]	ESR sp. ^g		(3)(4)
($^{80}\text{Se}^1\text{H}^-$)										
						$\text{I.P.} = 2.21 \text{ eV}^d$				JUL 1977
$^{80}\text{Se}^{16}\text{O}$										
		$\mu = 13.3274823_8$		$D_0^0 \leq 4.4_1 \text{ eV}^b$						OCT 1977
A large number of V shaded emission bands in the region $40000 - 55000 \text{ cm}^{-1}$ has tentatively been assigned to five or six systems with upper state vibrational frequencies ranging from ~ 940 to $\sim 1030 \text{ cm}^{-1}$ and lower state constants similar to those of the ground and first excited states of SeO .										
C_3 (0)	35484	581	H	3.5				$C_3 \rightarrow X_2$, R 35156	H	
C_2 ($^3\Pi_1$) (1)	35405	585	H	4.1				$C_3 \rightarrow X_1$, R 35313	H	(10)*
C_1 (2)	-	-	-	-				$C_2 \rightarrow X_2$, R 35075	H	
								$C_2 \rightarrow X_1$, R 35240	H	
B_2 $^3\Sigma^-$ {	1 (34376)	[517.5]	Z		[0.3417] ^{cd}	0.040 ₇	1.869	$B_2 \rightarrow X_2$, R 34012.2	Z	(1)(3)
B_1 {	0 ⁺ 34277.8	522.3	Z	3.9 ^a	[0.3332] ^d	0.029 ₂	1.907	$B_1 \rightarrow X_1$, R 34081.8	Z	
A'	(17364) ^e	885.2	H	5.8 ₅				$A' \rightarrow X$, ^f R 17349	H	(6)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{80}\text{Se}^{16}\text{O}$ (continued)										
A_3 (2) (16773)		[980]	H					$A_3 \rightarrow X_2$, V	16640 ^h	H
$A_2(^3\Pi_r)$ (1) 16458		996	H	7.0	$[(0.47_0)]^g$		$[(1.64)]$	$A_2 \rightarrow X_2$, V	16334 ^h	H
A_1 (0) 16144		994	H	6.5				$A_2 \rightarrow X_1$, V	16495 ^h	H
								$A_1 \rightarrow X_2$, V	16015 ^h	H
								$A_1 \rightarrow X_1$, V	16185 ^h	H
b $^1\Sigma^+$ 9723.5		838.8 ₃	(Z)	5.11	[0.4560]	(0.0035)	[8]	b $\rightarrow X_2$, R	9519.1	Z
a $^1\Delta$ (5300) ⁱ					[0.461]			b $\rightarrow X_1$, R	9685.4	Z
X_2 $3\Sigma^-$ {1 165.9		915.4 ₃ ^k	Z	4.52	0.4738 ^l	0.00339		ESR sp. ^j		(4)
X_1 {0 ⁺ 0		914.69 ^k	Z	4.52	0.4655	0.00323	5	ESR sp. ^m		(4)

Se^1H , Se^2H , Se^1H^- :

^aExtrapolation of the vibrational levels in $A \ ^2\Sigma^+$ assuming dissociation of this state into $^2\text{S} + ^1\text{D}$.

^bFrom Rydberg assignments of (5); doubtful.

^cFrom isotope relations between SeH and SeD .

^dFrom the photodetachment spectra of SeH^- and SeD^- (6).

^e Λ -doubling frequencies (3).

^f $\mu_{el} = 0.49 \text{ D}$ (4). ^{77}Se hf coupling (3).

^g $\mu_{el} = 0.483 \text{ D}$ (4). ^{77}Se hf coupling (3).

(1) Radford, JCP 40, 2732 (1964).

(2) Lindgren, JMS 28, 536 (1968).

(3) Carrington, Currie, Lucas, PRS A 315, 355 (1970).

(4) Byfleet, Carrington, Russell, MP 20, 271 (1971).

(5) Donovan, Little, Konstantatos, JCS FT II 68, 1812

(6) Smyth, Brauman, JCP 56, 5993 (1972). (1972).

SeO : ^aEmission bands with $v' > 2$ have not been observed, probably owing to predissociation. The limit is at $\sim 35600 \text{ cm}^{-1}$ above $X_1(v''=0)$.

^bFrom the predissociation in $B \ ^3\Sigma^-$; see ^a.

^cAverage of F_2 and F_3 , $B_0(F_3) - B_0(F_2) = +0.0052$.

^dRotational perturbations (1).

^e(6) give 17338.5 which does not agree with their v_{00} value. It is not clear whether X_1 or X_2 is the lower state of this system.

^f(6) considered the upper state to be b $^1\Sigma^+$, but v_{00} appears too high for this interpretation.

^gFrom P, Q head separations.

^hExtrapolated from bands having $v''=3$.

ⁱTheoretical estimate (9).

^j $\mu_{el}(a^1\Delta) = 2.01 \text{ D}$, from Stark effect on the ESR sp. (5).

(continued p. 589)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{78}\text{Se}^{32}\text{S}$		$\mu = 22.6698689$ $D_0^0 = (3.7) \text{ eV}^a$								JUL 1977
$B_2 \ 3\Sigma^- \begin{Bmatrix} 1 \\ 0^+ \end{Bmatrix}$ (28330)		[327.5 ₆]	^b	[0.1349]	^c		[2.348]	$B_2 \leftarrow X_2$, R	28011	(2)
$B_1 \ 3\Sigma^- \begin{Bmatrix} 1 \\ 0^+ \end{Bmatrix}$ 28248.2		[330.82] ^d z	(2.92)	0.1369 ^e	0.00121		2.331	$B_1 \leftarrow X_1$, R	28138.46 z	(2)
A 0^+ 27328.4		332.1 ^{df}	(2.66)	0.1186 ^{ef}	0.00095		2.504	$A \leftarrow X_1$, R	27216.5 (z)	(2)
$X_2 \ 3\Sigma^- \begin{Bmatrix} 1 \\ 0^+ \end{Bmatrix}$ 205 ^g		556.26 z	1.831	0.1812 ₁ ^h	0.00089	7	2.025 ₇			
$X_1 \ 3\Sigma^- \begin{Bmatrix} 1 \\ 0^+ \end{Bmatrix}$ 0		555.56 ^d z	1.848	0.1792 ₆	0.00076	6	2.036 ₇			
$^{80}\text{Se}^{32}\text{S}^-$		$\mu = 22.83624$								JUL 1977
A ($^2\Pi$)				The constants refer to SeS^- ions dissolved in KI crystals; from fluorescence spectra studied at 2 K (4).				$A \rightarrow X$,	17768.1	(2)(4)
X ($^2\Pi$) 0		468.9 ^a	1.66					Raman sp. ^b		(3)
								EPR sp. ^b		(1)
$^{32}\text{S}^{19}\text{F}$		$\mu = 11.9170627$ $D_0^0 \leq 3.3 \text{ eV}^a$								JUL 1977
$A_2 \ 2\Pi \begin{Bmatrix} 1/2 \\ 3/2 \end{Bmatrix}$		483 ^b H	2.6 ^b	(0.554) ^c	0.004		(1.59 ₈)	$A_2 \leftarrow X_2$, R	25205 H	(2)
$A_1 \ 2\Pi \begin{Bmatrix} 1/2 \\ 3/2 \end{Bmatrix}$		488 H	3.1					$A_2 \leftarrow X_1$, R	25606 H	
								$A_1 \leftarrow X_1$, R	24995 H	(2)*
$X_2 \ 2\Pi \begin{Bmatrix} 1/2 \\ 3/2 \end{Bmatrix}$ (401) ^d				[0.552174 ₀]			1.600574	Microwave sp. ^e		(4)
$X_1 \ 2\Pi \begin{Bmatrix} 1/2 \\ 3/2 \end{Bmatrix}$ 0								ESR sp.		(1)(3)

SeO (continued):

^kFrom $B \rightarrow X$ bands with $v'' \geq 5$; vibrational numbering confirmed by isotope studies.

^lAverage of F_2 and F_3 , $B_0(F_3) - B_0(F_2) = +0.0048$ (12).

^mHf coupling of ^{77}Se (4).

- (1) Barrow, Deutsch, PPS 82, 548 (1963).
- (2) Haranath, JMS 13, 168 (1964).
- (3) Haranath, IJPAP 3, 75 (1965).
- (4) Carrington, Currie, Levy, Miller, MP 17, 535 (1969).
- (5) Byfleet, Carrington, Russell, MP 20, 271 (1971).
- (6) Kushawaha, Pathak, SpL 5, 393 (1972).
- (7) Azam, Reddy, CJP 51, 2166 (1973).
- (8) Reddy, Azam, JMS 49, 461 (1974).
- (9) Barrow, Lemanczyk, CJP 53, 553 (1975).
- (10) Verma, Azam, Reddy, JMS 58, 367 (1975).
- (11) Verma, Azam, Reddy, JMS 65, 289 (1977).
- (12) Verma, Reddy, JMS 67, 360 (1977).

SeS: ^aEstimate based on a Birge-Sponer extrapolation of the ground state vibrational levels (2); see also (1).

^b $\Delta G(3/2) = 328.9_5$; see ^c.

^c $B_1 = 0.130_5$, $B_2 = 0.123$. Extensive perturbations by states having $\Omega = 1$ or 2.

^dVibrational numbering confirmed by isotope studies.

^eStrong mutual perturbations between B and A as well as other perturbations in B.

^fOnly $v' = 3$ and 4 have been analyzed, $\Delta G(7/2) = 310.79$.

^gEstimated from the magnitude of the Ω -type doubling; see ^h.

^h $B_e(F_3) - B_e(F_2) = +0.00063$.

SeS (continued):

(1) Drowart, Goldfinger, QR 20, 545 (1966).

(2) Ahmed, Barrow, JP B 7, 2256 (1974).

SeS⁻: ^aA Raman frequency of 464 cm^{-1} in KI has been observed by (3).

^bIn KI and NaI crystals.

(1) Vannotti, Morton, JCP 47, 4210 (1967).

(2) Rolfe, JCP 49, 4193 (1968).

(3) Holzer, Murphy, Bernstein, JMS 32, 13 (1969).

(4) Ikezawa, Rolfe, JCP 58, 2024 (1973).

SF: ^aFrom the predissociation in the $A_1 \leftarrow X_1$ bands; see ^c.

^bFrom the $A_2 \leftarrow X_2$ progression; slightly different numbers are obtained from $A_2 \leftarrow X_1$. The assignments of both progressions are tentative.

^cOnly $B_3 = 0.540$ and $B_5 = 0.532$ have been measured. Individual rotational lines are diffuse for $v' \geq 3$. Bands with $v' \geq 7$ are very diffuse.

^dBased on the assignments of progressions $A_2 \leftarrow X_2$ and $A_2 \leftarrow X_1$; from the ESR spectrum (1) derive $A_0 = -387 \pm 25$.

^e $\mu_{el}(v=0) = 0.79_4 \text{ D}$ (4); (3) obtain 0.87 D . Hfs parameter $a + \frac{1}{2}(b+c) = 428.6_0 \text{ MHz}$ (1)(4).

(1) Carrington, Currie, Miller, Levy, JCP 50, 2726 (1969).

(2) Di Lonardo, Trombetti, TFS 66, 2694 (1970).

(3) Byfleet, Carrington, Russell, MP 20, 271 (1971).

(4) Amano, Hirota, JMS 45, 417 (1973).

S^1H , S^2H :

- ^aFrom an extrapolation of the vibrational levels in $A^2\Sigma^+$ to the limit $1D+^2S$ (4); consistent with the observed predissociation in $A^2\Sigma^+$. Photoionization mass-spectrometry of H_2S (9) gives $D_0^0(S^1H) = 3.67$ eV (recalc. using updated auxiliary data). See also (20).
- ^bBoth D_0^0 and I.P. refer to the lowest existing molecular level, in agreement with definitions but contrary to the values given by (4) and (7), respectively, which refer to the zero-point of the Hill-Van Vleck expression for the ground state.
- ^cExtrapolation of a short Rydberg series (7).
- ^dThe ν_{00} values refer to the zero-point of the Hill-Van Vleck expression for the lower state and are exclusive of the J independent terms $-BA^2$ in the upper states, contrary to definitions normally adopted in these tables. Only the $X^2\Pi_{3/2}$ subbands have been observed.
- ^eFrom isotope shifts.
- ^fSpin splitting constant $\gamma_0 = +0.313$.
- ^gThe rotational lines of bands having $v' \geq 1$ are increasingly diffuse.
- ^h $\gamma_e = -0.022$.
- ⁱ $\beta_e = +0.60 \times 10^{-4}$.
- ^jObserved in absorption (flash photolysis of H_2S and D_2S) by (2)(4), in matrix absorption by (12), and in emission by (1)(11). Franck-Condon factors (3).
- ^k $A_0 = -376.96$ (2). On the basis of certain higher order corrections (15) gives $A_0 = -378.53$ (and $B_0 = 9.465$, $D_0 = 4.7 \times 10^{-4}$).
- ^lFrom the constants for SD (11).
- ^m Λ -doubling and hfs parameters (19).
- ⁿIn argon matrices at 20.4 K.
- ^oMolecular beam electric resonance study. The strongest Λ -

- doubling transitions in $2\Pi_{3/2}, J=3/2$ occur at 111.4862 ($F=1-1$) and 111.5452 MHz ($F=2-2$), in $J=5/2$ at 442.4781 ($F=2-2$) and 442.6277 MHz ($F=3-3$); these observations supersede earlier predictions (6)(16)(17) from EPR measurements.
- ^p $\mu_{el}(v=0) = 0.7580$ D (18)(19). Stark effect in EPR spectrum (8)(13a) yields the less accurate value 0.62 D. Predicted dipole moment function (20). Theoretical charge distributions (10).
- ^qFor EPR sp. of ^{33}SH and ^{33}S hf interaction see (14).
- ^rLarge electronic isotope shift.
- ^sSpin splitting constant $\gamma_0 = +0.163$. The lines of the 2-0 absorption band are diffuse.
- ^t $\gamma_e = -0.005$.
- ^u $\beta_e = +0.10 \times 10^{-4}$.
- ^v $A_0 = -376.75$ (2). Taking into account higher order corrections (15) derives $A_0 = -378.32$ (and $B_0 = 4.899$, $D_0 = 1.3 \times 10^{-4}$).
- ^wEstimates by (2) and (11).
- ^x $\mu_{el}(v=0) = 0.7571$ D (19).
- (1) Leach, CR 230, 2181 (1950).
- (2) Ramsay, JCP 20, 1920 (1952).
- (3) Nicholls, Fraser, Jarman, McEachran, ApJ 131, 399 (1960).
- (4) Johns, Ramsay, CJP 39, 210 (1961).
- (5) McDonald, JCP 39, 2587 (1963).
- (6) Radford, Linzer, PRL 10, 443 (1963).
- (7) Morrow, CJP 44, 2447 (1966).
- (8) Carrington, Levy, Miller, JCP 47, 3801 (1967).
- (9) Dibeler, Liston, JCP 49, 482 (1968).
- (10) Cade, Bader, Henneker, Keaveny, JCP 50, 5313 (1969).
- (11) Pathak, Palmer, JMS 32, 157 (1969).
- (continued p. 593)

S^1H , S^2H (continued):

- (12) Acquista, Schoen, JCP 53, 1290 (1970).
- (13) Uehara, Morino, JMS 36, 158 (1970).
- (13a) Byfleet, Carrington, Russell, MP 20, 271 (1971).
- (14) Miller, JCP 54, 1658 (1971).
- (15) Veseth, JMS 38, 228 (1971).
- (16) Brown, Thistlethwaite, MP 23, 635 (1972).
- (17) Tanimoto, Uehara, MP 25, 1193 (1973).
- (18) Meerts, Dymanus, ApJ 187, 145 (1974).
- (19) Meerts, Dymanus, CJP 53, 2123 (1975).
- (20) Meyer, Rosmus, JCP 63, 2356 (1975).

S^1H^+ : $a_{D_0^0}(S^1H) + I.P.(S) - I.P.(S^1H)$.
 $b_{A_0} = -216.5$ (1); see also (2).
 c Effective B value; for Λ -doubling constants see (1)(2).
 d From the "true" $B_0 = 7.47_2$ (2).
 e Lifetime $\tau(v=0) = 1090$ ns (5).
 f Effective value (1); the "true" origin is at 29911.28 cm^{-1} (2), the subband origins at 29675.55, 29912.81, 30141.71 cm^{-1} (1).
 g Spin splitting constants $\lambda_0 = +5.71_0$, $\gamma_0 = -0.16_5$ cm^{-1} .

- (1) Horani, Leach, Rostas, JMS 23, 115 (1967).
- (2) Horani, Rostas, Lefebvre-Brion, CJP 45, 3319 (1967).
- (3) Cade, CJP 46, 1989 (1968).
- (4) Liu, Legentil, Verhaegen, in "Selected Topics in Molecular Physics" (ed. Clementi), p. 19, Chemie GmbH (1972).
- (5) Brzozowski, Elander, Erman, Lyyra, PS 10, 241 (1974).

S^1H^- : a From $D_0^0(S^1H)$ and the electron affinities of S^1H and S .
 b From the photodetachment cross section (2).

- (1) Cade, JCP 47, 2390 (1967).
- (2) Steiner, JCP 49, 5097 (1968).

Si_2 : a From the observed predissociation in H (3) and thermochemical data [mass-spectrom.(2), recalcd.(3a)].
 $b_A = -28.2$.
 c Spin splitting constants $\lambda_0 = -6.68$ (slight J dependence), $\gamma_0 = +0.03_0$.
 $d_A = -22.6$ (from A'' and the observed subband origins).
 e The $^3\Pi_0$ subbands are essentially complete, but only fragments of the other subbands have been observed.
 f Average of the $^3\Pi_0$ and $^3\Pi_2$ subband origins. (1) gives 28059.1 which refers to the 0-1 rather than 0-0 band.
 g Also observed in rare gas matrices (3b)(5).
 h Extrapolated from the origins of the 1-0 and 2-0 bands. The 0-0 band ($\nu_H = 30771$) is completely diffuse.
 i Corrected vibrational numbering of (6).
 j The rotational lines of absorption bands having $v'=6$ are diffuse, indicating predissociation above 25877 cm^{-1} . Higher levels have not been observed.
 $k_A = -71.6$ (from the effective B values).
 l Progression of absorption bands in argon matrix, 34700 - 36300 cm^{-1} ; tentative interpretation (5).

- (1) Douglas, CJP 33, 801 (1955).
- (2) Drowart, De Maria, Inghram, JCP 29, 1015 (1958).
- (3) Verma, Warsop, CJP 41, 152 (1963).
- (3a) Verhaegen, Stafford, Drowart, JCP 40, 1622 (1964).
- (3b) Weltner, McLeod, JCP 41, 235 (1964).
- (4) Lagerqvist, Malmberg, PS 2, 45 (1970).
- (5) Milligan, Jacox, JCP 52, 2594 (1970).
- (6) Dubois, Leclercq, CJP 49, 3053 (1971).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
(28)Si⁽⁷⁹⁾Br		$(\mu = 20.6547281)$ Fragments of two other emission systems (30100 - 31500, 34900 - 36900 cm^{-1}) tentatively assigned to SiBr or SiBr ⁺ . Additional absorption bands at 45762, 46266, 46343, 46693, 47445 cm^{-1} .							SEP 1977		
(F)		[505] ^a	H					(F) ← X,	45017	H	(2)
E	(44560) 44521	552	H	1.5	Bands with $\nu'=1$ and 2 are diffuse.			E ← X,	V (44201) 44585	H	(9)
D	44017	[565] ^b	H					D ← X,	V 44088	H	(9)
C (² Π)	41060 41051	531 ^c	H	2.0				C ← X,	V 40690 ^c 41104 ^c	H	(9)
B (² Σ)	33572.4	571.2	H	2.4	de			B ↔ X,	V 33223.1 33645.1	H	(1)* (3)(5) (9)
B' (² Δ)	23911 23889	395	H	4				B' → X,	R 23473 23874	H ^Q	(7)
A (² Σ)	20937.6	250.3	H	0.5				A → X,	R (20428) 20850.9	H	(7)(8)
X ² Π_r	423.1 ^f 0	424.3	H	1.5	e						
(28)Si⁷⁹Br⁺											SEP 1977
A	29005.4	428.7	H	6.9				A → X, ^g	R 28950.5	H	(4)
X	0	535.8	H	1.6							
²⁸Si¹²C		$\mu = 8.39792238$ $D_0^0 = 4.64 \text{ eV}^a$ No spectra have yet been conclusively assigned to SiC. The following constants are from <u>ab initio</u> calculations (3):								AUG 1977 A	
a ¹ Σ^+	(6628)	(1018)		(0.695)			(1.70)				
A ³ Σ^-	(5597)	(606)		(0.556)			(1.90)				
X ³ Π_i	0 ^b	(983)		(0.606)			(1.82) ^b				

State	T _e	w _e		w _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References
									Design.	v ₀₀	
²⁸ Si ³⁵ Cl		μ = 15.5422824									SEP 1977
F									F← X,	45968 46179	H (12)
E									E← X,	45169 45375	H (12)
D	44943.9	659.4	H	3.8					D↔ X, V	44798.3 45005.8	H (1)(12)
C 2Π	41177.2 41165.7	674.2	H	2.20	[0.2888] ^a	0.0009	2.4	1.936	C↔ X, V	41039.9 41235.0	H (1)* (10) (12)
B' 2Δ	35631.0 ^b	511.1	Z	5.6	0.2618 ₇	0.00243	[3.59] ^c	2.035 ₂	B'↔ X, V _R	35411.25 ^d 35617.85 ₅	dZ (4)(6)* (9)

SiBr, SiBr⁺:

^aOnly two bands; it is not certain that they belong to the same system.

^bIt is possible that the $v'=1$ progression is in fact a separate system $D' \leftarrow X$.

^cVibrational numbering uncertain.

^dEmission bands with $v' > 2$ have not been observed.

^e(6) report the following rotational constants for the B-X bands: $B'_0 = 0.1771$, $B''_0(^2\Pi_{1/2}) = 0.1598$. See also (10) who give considerably different results.

^fFrom (5); (3) prefer a doublet separation of 418.0 cm^{-1} leading to slightly different constants.

^gBr isotope shifts clearly observed.

(1) Miescher, HPA 8, 587 (1935).

(2) Asundi, Karim, PIAS A 6, 281 (1937).

(3) Jevons, Bashford, PPS 49, 554 (1937).

(4) Kuznetsova, Kuzmenko, Kuzyakov, OS(Engl. Transl.) 24, 434 (1968).

SiBr, SiBr⁺ (continued):

(5) Kuznetsova, Kuzmenko, Kuzyakov, VMUK 23(3), 30 (1968).

(6) Kuznetsova, Kuzyakov, VMUK 24(6), 103 (1969).

(7) Kuznetsova, Kuzyakov, ZPS 10(3), 413 (1969).

(8) Rao, Haranath, JP B 2, 1381 (1969).

(9) Oldershaw, Robinson, TFS 67, 1870 (1971).

(10) Mishra, Khanna, IJP 46, 1 (1972).

SiC: ^aThermochemical value (mass-spectrom.)(1).

^b(2) assumes a $^1\Sigma$ ground state and estimates $r_e = 1.65 \text{ \AA}$ from an extrapolation to SiC of the shortening of Si-O, Si-N single bonds in the corresponding diatomic molecules.

(1) Verhaegen, Stafford, Drowart, JCP 40, 1622 (1964).

(2) Lovas, ApJ 193, 265 (1974).

(3) Lutz, Ryan, ApJ 194, 753 (1974).

SiC₂: ^aFrom (10); rotational analyses of a few additional sub-bands reported by (13).

(continued p. 597)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{28}\text{Si}^{35}\text{Cl}$ (continued)										
B $^2\Sigma^+$	34108.6	706.6 ^e	H 3.9 ^e	[0.2784] ^f	0.0017 ^f	1.8	1.971	B \leftrightarrow X, ^g V	33987.1 34193.6	Z (1)* (2)(3) (4)(5)(12) (16)
A $^2\Sigma$	23113.9	[294.9 ₅]	Z 0.73 H	0.1986	0.0007	[2.9] ^h	2.337	A \rightarrow X, R	22788.0 22994.7	Z (7)* (15)*
X $^2\Pi_r$	206.6 ⁱ ₀	535.60	Z 2.16 ₈ ^j	0.2561 ^k	0.0016	2.5 ^l	2.058			
$^{28}\text{Si}^{19}\text{F}$										
$\mu = 11.3148108$ $D_0^0 = 5.5_7 \text{ eV}^a$ I.P. = 7.2_8 eV^b										SEP 1977
Theoretical studies of low-lying valence states (22).										
I	[52834]							I \rightarrow X, V	52325 ^c 52489 ^c	H (5)
H ($^2\Sigma^+$)	(52095)	[1022]	H					H \rightarrow X, V	52098 ^c 52260 ^c	H (5)
(G)	(51941)	[1008]	H					(G \rightarrow X) V	51938 ^c 52098 ^c	H (5)
F	[52195]							F \rightarrow X, V	51685 ^c 51851 ^c	H (5)
E	[51650]							E \rightarrow X, V	51143 ^c 51302 ^c	H (5)
Unassigned V shaded bands in the region 47639 - 48325 cm^{-1} .										(4)
D $^2\Sigma^+$	47418.6	1003.2	5.64	0.625	0.005 ₅		1.54 ₄	D \rightarrow X, V	47491.4 ^d	(4)(5)*
D' $^2\Pi$	46612.5 ^e	1032.9	5.28	0.6329 ^f	0.0044		1.534 ₃	D' \rightarrow B, (12061.8)		(6)
								D' \rightarrow A, V	23912.6	(1)(6)
								UV ϵ bands		
								D' \rightarrow X, (46700.2)		(6)
C' $^2\Pi$	41964.7 ^g	1031.8	4.45	0.6376 ^f	0.0039		1.528 ₆	C' \rightarrow A, V	19264.5	(1)(6)
								Green ϵ b.		
								C' \rightarrow X, (42052.1)		(6)
C $^2\Delta$	39438.0 ^h	[878.38]	Z 5.8 ⁱ	0.60338 ^j	0.00539	[12.1] ^k	1.5713 ₇	C \rightarrow X, ^l V	39454.1 ₄	Z (2)(5)(11)*
								γ bands		

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{28}\text{Si}^{19}\text{F}$ (continued)										
B $^2\Sigma^+$	34561.5	1011.2 ₃	Z	4.825	0.62707 ^j	0.00462	10.1	1.5414 ₀	B \rightarrow A, ^m V 11850.8 ₄ Z B \rightarrow X, ⁿ V 34638.5 β bands	(5)* (1)* (2)(12)
a $^4\Sigma^-$	29805.06	863.16	Z	5.370	0.5786 ₂ ^o	0.00502	10.5	1.6046	a \rightarrow X, ^p η bands	29807.89 Z (7)* (20)*
A $^2\Sigma^+$	22858.3	718.5 ₈	Z	10.167 ^q	0.57839 ^{rj}	0.00941 ^s	15.7	1.6049 ₆	A ^t \leftrightarrow X, ^u R α bands	22787.64 Z (1)* (3)(5)
X $^2\Pi_r$	0 ^v	857.19	Z	4.735	0.5812 ₁ ^{wj}	0.00494	10.7	1.6011		

SiCl (continued):

^b $A_0 = +3.772$ [or -2.729 , see (6)].

^c $D_1 = 3.90 \times 10^{-7}$.

^dThe origins refer to the zero-point of the Hill-Van Vleck expression for the upper state and to the hypothetical $J''=0$ levels in the lower state.

^eCorrected using calculated head-origin separations (5).

^fAverage values of (3) and (16). See also (8)(11).

^gFranck-Condon factors (14).

^h $D_1 = 1.9 \times 10^{-7}$.

ⁱ $A_v = +207.21 - 0.32v$; small J dependent terms have been determined for $v=5 \dots 10$ (15).

^j $w_e y_e = +0.0053$.

^k Λ -type doubling $\Delta v(^2\Pi_{\frac{1}{2}}) = 0.005(J+\frac{1}{2})$ (15)(16).

^l $\beta_e = -0.09 \times 10^{-7}$.

(1) Jevons, PPS 48, 563 (1936).

(2) Barrow, Drummond, Walker, PPS A 67, 186 (1954).

(3) Ovcharenko, Tunitskii, Yakutin, OS(Engl. Transl.) 8, 393

(4) Thrush, Nature 186, 1044 (1960).

SiCl (continued):

(5) Ovcharenko, Kuzyakov, OS(Engl. Transl.) 13, 362 (1962).

(6) Verma, CJP 42, 2345 (1964).

(7) Sanii, Verma, CJP 43, 960 (1965).

(8) Cordes, Gehrke, ZPC (Frankfurt am Main) 51, 281 (1966).

(9) Ovcharenko, Kuzyakov, Tatevskii, OS(Engl. Transl.) Suppl. 2, 6 (1966).

(10) Ovcharenko, Kuzyakov, OS(Engl. Transl.) 20, 14 (1966).

(11) Mishra, Khanna, CS 38, 361 (1969).

(12) Oldershaw, Robinson, JMS 38, 306 (1971).

(13) Pandey, Upadhyaya, Nair, IJPAP 2, 36 (1971).

(14) Singh, Dube, IJPAP 2, 164 (1971).

(15) Singhal, Verma, CJP 42, 407 (1971).

(16) Rai, Singh, Upadhyaya, Rai, JP B 7, 415 (1974).

SiF: ^aThermochemical value (mass-spectrom.) (9).

^bExtrapolation of a short Rydberg series B,D,H,... (5); the value of (5) has been slightly modified in accordance with the definition of the I.P.. (9) give an electron impact ap- (continued p. 599)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{28}\text{Si}^1\text{H}$		$\mu = 0.97278226$ $D_0^0 \leq 3.06_0 \text{ eV}^a$ I.P. $\leq 8.04 \text{ eV}^b$							AUG 1977	
E	$^2\Sigma^+$ [53411.2]	Only $v=0$ observed	[7.528]		[3.92]	[1.517 ₂]	E \leftarrow X, V	52399.19 Z	(10)*	
D	$^2\Delta$ [49522.1]	Only $v=0$ observed	[7.90] ^c			[1.48 ₁]	D \leftarrow X, V	48510.1 Z	(5)(10)*	
B	$^2\Sigma^+$ [31842.2]	Only $v=0$ observed	[6.62] ^{de}			[1.61 ₈]	B \leftarrow X, R	30830.2 ^d Z	(5)* (13)	
C	$^2\Sigma^+$ [31832.4]	Only one level observed	[1.17] ^d			[3.8 ₅]	C \leftarrow X, R	30820.4 ^d Z	(5)(13)	
"Slightly diffuse" weak absorption bands in the region 25600 - 26700 cm^{-1} .										(4)
A	$^2\Delta$ 24300.4 ^f	1858.90 ^g Z 99.17 ₅	7.4664 ^g	0.3445 ^h	[5.24] ⁱ	1.5234 ₇	A ^j \leftrightarrow X, ^k R	24193.04 Z	(1)* (2)(5)* (6)(10)	
X	$^2\Pi_r$ 0 ^l	2041.80 ^g Z 35.51	7.4996 ^{gm}	0.2190 ⁿ	[3.97]	1.5201 ₀	Extensive theoretical calculations ^o			

$\text{Si}^1\text{H}, \text{Si}^2\text{H}_2$

^aFrom the predissociation in B $^2\Sigma^+$ assuming dissociation into $^1\text{D} + ^2\text{S}$ at the predissociation limit (5). According to (2) extrapolation of the vibrational levels in A $^2\Delta$ gives very nearly the same limit.

^bFrom $D_0^0(\text{Si}^1\text{H})$, I.P.(Si), and $D_0^0(\text{Si}^1\text{H}^+)$ (12).

^cIncreasing diffuseness with increasing N on account of predissociation.

^dDeperturbed constants of (13) whose T_0 values correspond to $v_{00} + 1079.5$ [see (6)]. As in similar cases, v_{00} refers to the zero-point of the Hill-Van Vleck expression for the ground state. Interaction parameter $H_{B,C} = 16.1 \text{ cm}^{-1}$. The v numbering of the C level is uncertain.

^eStrongly predissociated above N=2.

^f $A_0 = 3.58$, $A_1 = 3.11$, $A_2 = 2.59$ (6). Discussion of second order spin-orbit splittings (14).

^gRecalculated (10) from data for $v=0, 1, 2$ (6).

^h $\gamma_e = -0.0418_5$.

ⁱ $D_1 = 6.08 \times 10^{-4}$, $D_2 = 7.36 \times 10^{-4}$.

^j(11) gives a radiative lifetime of 0.7 μs for both SiH and SiD corresponding to $f_{00} = 0.0037$ (16); see also (17).

^kPotential functions, Franck-Condon factors (15)(16). | (6).

^l $A_0 = +142.83$, $A_1 = +143.43$, $A_2 = +144.04$. Slight J dependence

^mFor Λ -doubling constants ($p_0 = 0.0819$, $q_0 = 0.00831$) see (6) (20); the extrapolated splitting of the $v=0$, $J=\frac{1}{2}$ level is $\Delta v_{fe} = +0.0978 \text{ cm}^{-1}$ ($2932 \pm 20 \text{ MHz}$) (20); ab initio calculations (19) predict 0.1057 cm^{-1} (3168 MHz).

ⁿ $\gamma_e = +0.0017$.

^oHartree-Fock wavefunctions and energies (8), charge distributions (9), spectroscopic constants (18).

(References on p.601)

SiF (continued):

pearance potential of 7.5 eV; ab initio calculations predict 7.4 eV (19).

^cQ₁ and P₂ heads. (The head designations in Table 4 of (5) are erroneous.)

^dAccording to (4) the 0-0 Q₁ and P₂ heads are at 47569.2 and 47408.9 cm⁻¹, respectively.

^eA ≈ 0.

^f(6) give Λ-doubling constants.

^gA = 16.5₄.

^h(11) assume a regular state with A₀ = +2.46 and A₁ = +2.35.

ⁱFrom (5); Pekeris' relation gives 7.01 (11).

^jRKR potential curves (10).

^kD₁ = 13.5 × 10⁻⁷.

^lFranck-Condon factors (14).

^mFranck-Condon factors (18).

ⁿFranck-Condon factors (13)(18); variation of transition moment with r (16).

^oSpin splitting constants λ₀ = +0.274, λ₀^{*} = +0.00188; (20) find that the ⁴Σ levels can be fitted with one g-type doubling parameter γ rather than the two proposed by (8) to account for earlier results by (7).

^pTwo short 0-0 sequences of headless bands centred at 29728 and 29890 cm⁻¹. Franck-Condon factors (21).

^qω_eν_e = +0.157.

^rSpin splitting constant λ₀^{*} = -0.0062₅.

^sω_e = +0.00013.

^tRadiative lifetime τ(ν=0) = 0.23 μs (23).

^uObserved in absorption in a shock tube experiment (15). Franck-Condon factors (18). Electronic transition moment (15), variation with r (17).

^vA₀ = +161.88, A₁ = +162.04, A₂ = +162.19 (20), see also (11). Small J dependent terms have also been determined.

^wΛ-doubling constants p₀ = -0.00299 [i.e. Δν_{fe}(²Π_{1/2}) ≈ -0.0030(J+½)], q₀ = -1.06 × 10⁻⁵ (20).

(1) Johnson, Jenkins, PRS A 116, 327 (1927).

(2) Asundi, Samuel, PIAS A 3, 346 (1936).

(3) Eyster, PR 51, 1078 (1937).

(4) Dovell, Barrow, PPS A 64, 98 (1951).

(5) Johns, Barrow, PPS 71, 476 (1958).

(6) Barrow, Butler, Johns, Powell, PPS 73, 317 (1959).

(7) Verma, CJP 40, 586 (1962).

(8) Hougen, CJP 40, 598 (1962).

(9) Ehlert, Margrave, JCP 41, 1066 (1964).

(10) Singh, Rai, IJPAP 4, 102 (1966).

(11) Appelblad, Barrow, Verma, JP B 1, 274 (1968).

(12) Singh, Singh, CS 37, 8 (1968).

(13) Mohanty, Singh, IJPAP 7, 109 (1969).

(14) Singh, Maheshwari, IJPAP 7, 708 (1969).

(15) Kuzyakov, Ovcharenko, Kuz'menko, Kurdyumova, ZPS 12(3), 555 (1970).

(16) Kuz'menko, Kuzyakov, Smirnov, ZPS 13(4), 616 (1970).

(17) Kuz'menko, Smirnov, Kuzyakov, VMUK 25(3), 357 (1970).

(18) Wentink, Spindler, JQSRT 10, 609 (1970).

(19) O'Hare, Wahl, JCP 55, 666 (1971).

(20) Martin, Merer, CJP 51, 634 (1973).

(21) Singh, IJPAP 13, 204 (1975).

(22) Bialski, Grein, JMS 61, 321 (1976).

(23) Davis, Hadley, PR A 14, 1146 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{28}\text{Si}^2\text{H}$										
		$\mu = 1.87884152$		$D_0^0 \leq 3.09_5 \text{ eV}^p$						AUG 1977
E	$^2\Sigma^+$	[53111.85]		[3.9161]		[1.028]	[1.5136 ₅]	E \leftarrow X,	V 52381.75 Z	(10)*
D	$^2\Delta$	[49255.6]		[4.00 ₉]		[1]	[1.496]	D \leftarrow X,	V 48525.5 ^q Z	(5)*
C	$^2\Sigma^+$	[31728.2]		[1.09] ^r			[2.8 ₇]	C \leftarrow X,	R 30998.1 ^r Z	(13)
B	$^2\Sigma^+$	[31634.9]		[3.703] ^{rs}		[3.4] ^r	[1.556 ₆]	B \leftarrow X,	R 30904.8 ^r Z	(5)* (13)
A	$^2\Delta$	24313.8 ^t	1328.08 ^g Z 48.11	3.8680 ^g	0.1318 ^u	[1.379] ^v	1.5230 ₄	A \leftrightarrow X,	R 24235.66 Z	(5)* (6)
X	$^2\Pi_r$	0 ^w	1469.32 ^g Z 18.23	3.8840 ^{gx}	0.0781 ^y	[1.054]	1.5198 ₉			
$^{28}\text{Si}^1\text{H}^+$										
				$D_0^0 = 3.17 \text{ eV}^a$						AUG 1977
A	$^1\Pi$	25846.1	[390.17] Z (72.0) ^b	4.9125 ^c	0.7667	[19.92] ^d	1.8782	A \rightarrow X, ^{eh}	R 25025.20 Z	(1) ^f
X	$^1\Sigma^+$	0	2157.17 Z 34.24	7.6603	0.2096 ^g	3.83 ^g	1.5041			
$^{28}\text{Si}^1\text{H}^-$										
		$D_0^0 \leq 2.95_2 \text{ eV}^a$		I.P. = 1.277 eV ^b						AUG 1977
b	$^1\Sigma^+$	[8460]	(2100) ^c				(1.50) ^c			
a	$^1\Delta$	[4580]	(2100) ^c				(1.50) ^c			
X	$^3\Sigma^-$	[0]	(2175) ^c				(1.474) ^c			
$^{28}\text{Si}^{127}\text{I}$										
		$\mu = 22.9233294$		$D_0^0 = 3.0 \text{ eV}^a$						SEP 1977
		Unassigned absorption bands in the region 41500 - 43600 cm^{-1} .								
(E)		Diffuse bands, assignment uncertain.								
D								F \leftarrow X ₁ ,	V 44995 H	(4)
C	42711	486	H 3.5	v=2 diffuse.				(E \leftarrow X)	(44104)	(4)*
B	$^2\Sigma$	32380.3	471.7	H 0.9	All levels predissociated. ^b			D \leftarrow X ₁ ,	V 42859 H	(4)*
A	$^2\Sigma$	21204.9	208.6	H 1.66 ^c	d			C \leftarrow X ₁ ,	V 42772 H	(4)*
a	($^4\Sigma_{\frac{1}{2}}^-$)	x+20289.7	275.7	H 5.6	[(0.118)] ^e		[(2.50)]	B \leftarrow X ₁ ,	V 32434.3 H	(1)(3)*
								A \leftarrow X ₁ ,	R 21127.2 H	(3)*
								a \leftrightarrow X ₂ , ^f	R 20246.9 H	(2)* (3)*

Si¹H, Si²H (continued):

- ^pFrom the value for Si¹H, confirmed by the observed pre-dissociation in B ²Σ⁺.
- ^qRecalculated from the data of (5).
- ^rDeperturbed constants of (13) whose T₀ values correspond to v₀₀ + 797.50 [see (6)]. Interaction parameter H_{B,C} = 5.87 cm⁻¹. See d.
- ^sIncreasing linewidth above N=8 indicating predissociation.
- ^tA₀ = 3.45, A₁ = 3.42, A₂ = 2.14 (6); see also (14).
- ^uγ_e = -0.0101.
- ^vD₁ = 1.524 x 10⁻⁴, D₂ = 1.708 x 10⁻⁴.
- ^wA₀ = +142.73, A₁ = +143.10, A₂ = +143.76; slight J dependence
- ^x(6) give Λ-doubling constants (p = 0.039, q = 0.0024). | (6).
- ^yγ_e = -0.0009.
- (1) Rochester, ZP 101, 769 (1936).
 - (2) Douglas, CJP 35, 71 (1957).
 - (3) Barrow, Deutsch, PCS (1960), p. 122.
 - (4) Thrush, Nature 186, 1044 (1960).
 - (5) Verma, CJP 43, 2136 (1965).
 - (6) Klynning, Lindgren, AF 33, 73 (1966).
 - (7) Cade, PPS 91, 842 (1967).
 - (8) Cade, Huo, JCP 47, 649 (1967).
 - (9) Cade, Bader, Henneker, Keaveny, JCP 50, 5313 (1969).
 - (10) Herzberg, Lagerqvist, McKenzie, CJP 47, 1889 (1969).
 - (11) Smith, JCP 51, 520 (1969).
 - (12) Douglas, Lutz, CJP 48, 247 (1970).
 - (13) Bollmark, Klynning, Pagès, PS 3, 219 (1971).
 - (14) Veseth, Physica 56, 286 (1971).
 - (15) Rao, Lakshman, Physica 56, 322 (1971).
 - (16) Smith, Liszt, JQSRT 11, 45 (1971).
 - (17) Grevesse, Sauval, JQSRT 11, 65 (1971).
 - (18) Meyer, Rosmus, JCP 63, 2356 (1975).

Si¹H, Si²H (continued):

- (19) Wilson, Richards, Nature 258, 133 (1975).
- (20) Freedman, Irwin, AA 53, 447 (1976).

- Si¹H⁺: ^aFrom a short extrapolation of the vibrational levels in
- ^bEstimated from Pekeris' relation (1). | A ¹Π (1).
- ^cFrom average B_v values for the two Λ-doubling components; B(P,R) - B(Q) = +0.0062 and +0.0156 for v=0 and 1, resp..
- ^dD₁ = 17.89 x 10⁻⁴. In both v=0 and 1, rotational levels having J ≥ 9 cannot be represented by short power series in J(J+1).
- ^eAlso observed in the solar spectrum (2). On the basis of this observation (3) obtain f₀₀ = 0.0005; see, however, (5).
- ^fTable IV as well as eqn.[3] and eqn.[5] of (1) contain several errors which were later corrected in an unpublished erratum.
- ^gγ_e = +0.0045, β_e = -0.05 x 10⁻⁴.
- ^hPotential functions, Franck-Condon factors (4)(5).
- (1) Douglas, Lutz, CJP 48, 247 (1970).
 - (2) Grevesse, Sauval, AA 2, 232 (1970).
 - (3) Grevesse, Sauval, JQSRT 11, 65 (1971).
 - (4) Rao, Lakshman, Physica 56, 322 (1971).
 - (5) Liszt, Smith, JQSRT 12, 947 (1972).
- Si¹H⁻: ^aFrom D₀⁰(Si¹H) and the electron affinities of Si and Si¹H.
- ^bFrom laser photoelectron spectroscopy (1). See also ref. (7) of Si¹H.
- ^cFranck-Condon analysis of the photodetachment sp. (1).
- (1) Kasdan, Herbst, Lineberger, JCP 62, 541 (1975).
- SiII: ^aExtrapolation of the vibrational levels in A ²Σ (3). An upper limit of 4.02 eV follows from the prediss. in B ²Σ. (continued p. 603)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{28}\text{Si}^{127}\text{I}$ (continued)										
$X_2 \quad 2\Pi_{3/2}$	x^g	359.0	H 1.1							
$X_1 \quad 2\Pi_{1/2}$	0	363.8	H 1.2 ₅	$[(0.123)]^h$			$[(2.45)]$			
$^{28}\text{Si}^{14}\text{N}$									SEP 1977	
$\mu = 9.3321339_g$										
The emitter of the Woods band at 26017 cm^{-1} (3) has been shown (11) to be SiO^+ and not SiN as suggested by (9).										
L $2\Pi_i$	$a+(32661)^a$	$[718]^b$	H		$[0.549]^b$		$[1.814]^b$	L \rightarrow A, R 32491^b 32508^b	H (14)	
D $2\Pi_i$	$a+27865.6^c$	699.3_3	Z 3.48		0.5238^d	0.0041	1.857_1	D \rightarrow A, R 27693.8	Z (1)(6)(13) (14)*	
K 2Σ	$a+25718.2$	1142^b	Z 11.5		0.677_5^b	0.005	1.633^b	K \rightarrow A, V 25765.7^b	Z (14)*	
B $2\Sigma^+$	24299.2_1	1031.03	Z 16.85^e		0.7238^{fgh}	0.01048	1.579_8	B \leftrightarrow X, ⁱ R 24236.4_7	Z (1)(2)* (4) (10)(14)	
A $2\Pi_i$	a^{jk}	1044.4_1	Z 6.20^l		0.67516	0.00538	1.6357_0			
X $2\Sigma^+$	0	1151.3_6	Z 6.47^m		0.7311^{noh}	0.00565	1.571_9			

SiN: ^a $A \approx -72$.

^bVibrational numbering unknown; the lowest observed level is arbitrarily assumed to have $v=0$.

^cThe observed spin-orbit coupling constants vary from $A_3 = -60.42$ to $A_7 = -63.49$ (14).

^dPerturbations in $v=3$ by a Σ state (13)(14).

^e $w_e y_e = +0.15$, $w_e z_e = -0.011$.

^f(11) give the spin splitting constant $\gamma_0 = +0.0020$ but (14) change this to -0.0034 .

^gNumerous perturbations; for a summary see (14).

^hPotential curves (7), see also (14).

ⁱThe 0-0 sequence was wrongly attributed to SiO^+ by (8), see the correction by (9). Measured relative intensities, Franck-Condon factors, r dependence of the transition moment (5)(12).

^j(14) estimate $a \approx 8000$.

^kThe observed spin-orbit coupling constants $[A_1 \dots A_5]$ (14) are approximately given by $A_v = -89.54 + 0.27(v + \frac{1}{2})$.

^l $w_e y_e = -0.011$.

^m $w_e y_e = -0.007$.

SiN (continued):

ⁿ(11) give the spin splitting constant $\gamma_0 = +0.0153$ [see also (9)(10)] but (14) change this to -0.0172 .

^oA small perturbation in $v=8$ probably arises from interaction with A $^2\Pi$ (14).

- (1) Mulliken, PR 26, 319 (1925).
- (2) Jenkins, de Laszlo, PRS A 122, 103 (1929).
- (3) Woods, PR 63, 426 (1943).
- (4) Thrush, Nature 186, 1044 (1960).
- (5) Stevens, Ferguson, CJP 41, 240 (1963).

- (6) Schofield, Broida, PP 4, 989 (1965).
- (7) Singh, Rai, IJPAP 4, 102 (1966).
- (8) Nagaraj, Verma, CJP 46, 1597 (1968).
- (9) Dunn, Rao, Nagaraj, Verma, CJP 47, 2128 (1969).
- (10) Dunn, Dunn, CJP 50, 860 (1972).
- (11) Singh, Bredohl, Remy, Dubois, JP B 6, 2656 (1973).
- (12) Gohel, Shah, IJPAP 13, 162 (1975).
- (13) Linton, JMS 55, 108 (1975).
- (14) Bredohl, Dubois, Houbrechts, Singh, CJP 54, 680 (1976).

SiI (continued):

^bThe bands become progressively more diffuse with increasing v' (3).

^c $w_e y_e = +0.079$, $w_e z_e = -0.0055$.

^dOnly the 7-0 and 8-0 bands of $A \leftarrow X_1$ have been analyzed (3), $B' \approx 0.085$. Of the six expected branches only four have been observed; R_{11} and Q_{P21} (i.e. R_{ee} and P_{ff}) lines are absent. Extensive perturbations by levels of a $^4\Sigma_{\frac{1}{2}}^-$ state; see ^e.

^eAs a full rotational analysis of the emission bands [called $A' \rightarrow X$ by (3) and $A \rightarrow X$ by (2)] was not possible, the nature of the a state is not known. (3) suggests that this is the same $^4\Sigma_{\frac{1}{2}}^-$ state whose higher vibrational levels ($\Delta G \approx 176$, $B \approx 0.097$) have been identified in perturbations of A $^2\Sigma(v=7,8)$.

^fA much weaker system reported by (2) at 650 cm^{-1} to the red of the main system was not confirmed by (3). Transitions to or from $X_1 \ ^2\Pi_{\frac{1}{2}}$ have not been observed.

^g(3) assumes $x \approx 700 \text{ cm}^{-1}$. Tentative assignments of weak absorption bands would give $x = 649$ (3) or 757 cm^{-1} (1).

^hEstimated by assuming the same percentage decrease in bond length from HSiI to SiI as from HSiCl to SiCl (3). The rotational analysis of the $A \leftarrow X_1$ 7-0 and 8-0 bands gives $B'' - |p''|/2 = 0.10987$ and $D'' = 2.1 \times 10^{-7}$.

- (1) Oldershaw, Robinson, TFS 64, 2256 (1968).
- (2) Lakshminarayana, Haranath, JP B 3, 576 (1970).
- (3) Billingsley, JMS 43, 128 (1972).
- (4) Oldershaw, Robinson, JMS 44, 602 (1972).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{28}\text{Si}^{16}\text{O}$		$\mu = 10.1767076_1$ $D_0^0 = 8.26 \text{ eV}^a$ I.P. = 11.4_3 eV^b								AUG 1977 A
		Theoretical potential curves and spectroscopic constants for the ground and several valence-excited states (19a)(46).								
P	$1\Sigma^+(5p6)$ 82019	[1121.5]	Z	[0.692]	c		[1.54 ₇]	P \leftarrow X, ^d	R 81960.3	Z (24)*
O	1Π [82208.1]			[0.556]	e		[1.72 ₆]	O \leftarrow X, R	81588.8	Z (24)
N	1Π (81232)	[(1024)]		[0.635]	f		[1.61 ₅]	N \leftarrow X, R	81124.8	Z (24)
M	1Π 81203	[833]		[0.640]	g		[1.60 ₉]	M \leftarrow X, ^d	R 81000.5	Z (24)
L	$1\Sigma^+(5s6)$ 80783	[1102.2]	Z	[0.701]	h		[1.53 ₇]	L \leftarrow X, ^d	R 80715.3	Z (24)*
K	$1\Sigma^+$ 78369	[905.8]	Z	[0.615]	i		[1.64 ₁]	K \leftarrow X, ^d	R 78202.6	Z (24)
J	1Π (4p π) 76381	[1146]		[0.6983]	j		[1.540 ₂]	J \leftarrow X, ^d	R 76334.3	Z (24)*
h	$3\Pi_i$ (70790) ^k	(431) ^k		$B_1 \approx 0.589^k$			$r_1 \approx 1.67_7$			(33)
I	1Π (70510)	[878.9]	Z	[0.614]	ℓ		[1.64 ₃]	I \leftarrow X, R	70333.7	Z (24)
H	$1\Sigma^+(4p6)$ 69727	[1109.2 ₅]	Z	0.7146	0.0094 ^m		1.522 ₅	H \leftarrow X, ^d	R 69662.2 ₆	Z (24)* (33)*
G	1Π (69670)	[862.8 ₈]	Z	[0.6292]	ℓ	[1.2]	[1.622 ₆]	G \leftarrow X, R	69483.0 ₆	Z (24)*
F	$1\Sigma^+(4s6)$ 68532.0	1120.0 ₀ ⁿ	Z	7.34 ₅ ⁿ	o		[1.545 ₂]	F \leftarrow X, ^d	R 68470.9 ₀	Z (2)* (24)*
		Many unidentified emission bands in the region 21800 - 31500 cm^{-1} .								(47)
g	$3\Sigma^+(4s6)$ [68091.4]			[0.71588]		[1.42]	[1.5211 ₆]	g \rightarrow b, V	$\begin{cases} 33567.9_5 \\ 33639.0_1 \\ 33711.5_9 \end{cases}$	Z (35)*
f	$3\Pi_i$ $\begin{cases} 59283.1 \\ 59260.8 \\ 59236.8 \end{cases}$	488.4 ^p	3.4	0.586 ^p	0.014 ₅	3	1.68 ₁	f \rightarrow b, R	$\begin{cases} 25146.6 \\ 25051.7 \\ 24956.7 \end{cases}$	H (18)* (37) H (47)*
c	$3\Sigma(+)$ 57551.3	949.10	H 17.30	0.6841 ^q	0.0079	1.7	1.556 ₁	c \rightarrow b, V _R	$\begin{cases} 23498.0_5 \\ 23569.1_1 \\ 23641.6_9 \end{cases}$	Z (11)* (35) Z (47)
E	$1\Sigma^+$ 52860.9	675.52	Z 4.204	0.54727 ^r	0.00555 ^s	1.434 ^t	1.7397 ₈	E ^u \leftrightarrow X, ^v	R 52578.31	Z (15)* (36) (47)*

SiO: ^aAverage of several thermochemical determinations; see the summary in the Appendix of (30), also (5)(25).
^bAverage of the values obtained on the assumption that F,L,... and H,P,... are the first members of two Rydberg series converging to $X\ ^2\Sigma^+$ of SiO^+ (24)(32). The electron impact appearance potential is 11.5₈ eV (8)(16).
^cOnly v=0 and 1 observed; $B_1 = 0.703$. Both levels are perturbed.
^dCorresponding data for $Si^{18}O$ and confirmation of the vibrational numbering (32).
^eOnly one strongly perturbed level observed, vibrational numbering uncertain.
^fv=1 diffuse. Vibrational numbering doubtful.
^gOf the two observed levels only v=0 has been partially analyzed.
^hv=0 strongly perturbed. Only fragments of the 1-0 band observed, $B_1 = 0.67$. The 2-0 band at 1207 Å (82850 cm⁻¹) has very broad lines.
ⁱHigher ΔG and B_v values (v ≤ 5) are irregular.
^jv=0 strongly perturbed; v=1 observed but not analyzed.
^kv=1 observed in a perturbation of $H\ ^1\Sigma^+(v=1)$; $A_1 \approx -36$. Slightly different constants are given by (48a): $T_e = 70826$, $A_1 = -33.2$, $\omega_e = 414$, $B_1 = 0.5763$.
^lThe G and I states interact strongly. Higher ΔG and B_v values are irregular. The vibrational assignments of (24) have been revised by (32) to account for isotope shifts; the vibrational numbering of the I state is still in doubt, see (48a). The linewidth in bands labelled G-X (according to the new assignments of (32)] increases with v'. G(v=3) is perturbed by a $^3\Sigma^+$ state (probably v=4 of g $^3\Sigma^+$) having $B = 0.687$, $T_v = 71937\text{ cm}^{-1}$.

^mv=1 perturbed by h $^3\Pi_1(v=1)$, see ^k.
ⁿThese constants represent only v=0,1,2. There are vibrational perturbations for higher v which may also affect the lower levels.
^o $B_1 = 0.6888$, $B_2 = 0.6785$.
^pApproximate constants from a partial analysis of the 1-0, 3-0, 4-0 bands (18)(37); vibrational constants confirmed by (47). The v=0 level is perturbed (37); according to (48) the $^3\Pi_1$ component interacts strongly with A $^1\Pi(v=23)$. (48) give constants which differ considerably from those of (37).
^qSpin splitting constants for v=1: $\lambda = 0.298$, $\gamma = -0.002$ (11).
^rRKR potential curve (45); notice that the total energies of the potential curves calculated by (45) are unreliable since the T_e values used by them are, in fact, T_{00} values.
^s $\gamma_e = +0.000022$.
^t $\beta_e = +0.018 \times 10^{-6}$.
^uRadiative lifetime $\tau(v=1...7) = 10.5\text{ ns}$ (23). These authors have calculated Franck-Condon factors and f values for bands of the v'-0 progression and have determined the r dependence of the transition moment.
^vA new emission system reported by (22) has been shown (36) to be part of the E→X system with high v' and v"; see also (47).

(References on p.607)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{28}\text{Si}^{16}\text{O}$ (continued)										
A 1_{Π}	42835.4	852.8	Z 6.43 ^a	0.6307 ^{bc}	0.00660	1.43	1.620 ₆	$A^d \leftrightarrow X, ^e R$	42640.71 Z	(1)* (9) (17)* (38)* (47)* (49)*
D 1_{Δ}	38823 ^f	730		0.553 ₈ ^c	0.0051 ₆		1.729			
C 1_{Σ^-}	38624 ^f	740		0.555 ₅ ^c	(0.005 ₂)		1.727			
e 3_{Σ^-}	38309 ^f	748		0.556 ₃ ^c	0.0051 ₅		1.726			
d 3_{Δ_r}	36487 ^{fg}	767		0.563 ₁ ^c	(0.005 ₂)		1.715			
b $\begin{cases} 3_{\Pi_2} \\ 3_{\Pi_1} \\ 3_{\Pi_0} \end{cases}$	34018.5	1013.8	(Z) 7.5 ₇	$[0.68920]^i$	0.0044 ₀	$[2.2_2]$	1.5624	$b \rightarrow X, \quad R \begin{cases} 33904.2_0 \text{ Z} \\ 33833.1_4 \text{ Z} \\ 33760.5_6 \text{ Z} \end{cases}$		(27)(29)(39) (51)
	33947.4 ^h			$[0.67607]^{ic}$		$[1.2_5]$				
	33874.8			$[0.66386]^i$		$[0.50]$				
a 3_{Σ^+}	(33630)	(790) ^j	(4.1) ^j	(0.57) ^{jc}	(0.0052) ^j		(1.70) ^j	$a \rightarrow X, \quad R$	33409 H	(29)(39)(51)
X 1_{Σ^+}	0	1241.55 ₇	Z 5.966 ^k	0.7267512 ^c	0.0050377 ^l	0.980	1.509739	Rot.-vibr. sp. ^m		(19)(26)
								Rotation sp. ⁿ		(7)(31)(34) (50)
								Mol. beam rf el. reson. ^o		(12)(28)

SiO: ^a $w_e v_e = +0.0238$ (49).

^bThe A 1_{Π} state is extensively perturbed by levels of d 3_{Δ} , e 3_{Σ^-} , c 1_{Σ^-} , D 1_{Δ} ; see (49) who give a very detailed analysis of these perturbations for $^{28}\text{Si}^{16}\text{O}$ and $^{28}\text{Si}^{18}\text{O}$. Selective enhancement of perturbed and corresponding "extra" lines in emission under fast pumping conditions (44).

^cRKR potential energy curves for the eight lowest states (49); see also (4)(45) and ^r on p.605 concerning the results of (45).

^dRadiative lifetime $\tau = 9.6$ ns [phase-shift method (20)] corresponding to $f_{el} = 0.13$; see also (10). Considerably

smaller f values have been derived by (6)(13); for a summary of reported f values see (46) whose theoretical calculations predict $\tau = 32$ ns.

^eFranck-Condon factors (3)(21)(48a). Isotope shifts for $^{29}\text{Si}^{16}\text{O}$ and $^{30}\text{Si}^{16}\text{O}$ (42)(47).

^fAll constants for these states derived from perturbations in A 1_{Π} (1)(49).

^g $A = +8$. There is a strong spin-orbit interaction between 3_{Δ_2} and 1_{Δ_2} which causes a large asymmetry in the spin splitting of d 3_{Δ} (49).

^h $A_0 = +73.19$, $A_1 = +73.02$ (11).

ⁱEffective B_0 values (35); using instead sums of $\Delta_2 F(J)$ for

SiO (continued):

the three components (11) obtain $B_0 = 0.6766_g \cdot \Lambda$ -type doubling in $^3\Pi_0$ and $^3\Pi_1$ (35).

^jPredicted constants (49); see also (19a)(46). Only $v'=0$ has been observed in chemiluminescence. From partially resolved rotational structure (51) derive $B_0 \approx 0.59$.

^k $w_e y_e = +0.0054557$; these are the constants of (36)(49) which are very similar to the old constants of (1) and the more recent ones of (26) (rotation-vibration sp.); see also (14)(17).

^l $y_e = +2.35 \times 10^{-6}$ (50).

^mObserved in late-type stars (26)(43).

ⁿSeveral microwave lines have been observed in interstellar space and some extended stellar atmospheres, see e.g. (40)(41). Maser action is prevalent.

^o $\mu_{el}(v) = 3.0882 + 0.0197(v + \frac{1}{2})$ D for $v \leq 3$ (12); for g_J factors ($-0.1536 \mu_N$ for $v=0$) and other magnetic properties see (28), also (31).

- (1) Lagerqvist, Uhler, AF 6, 95 (1952).
- (2) Barrow, Rowlinson, PRS A 224, 374 (1954).
- (3) Nicholls, JRNBS A 66, 227 (1962).
- (4) Nair, Singh, Rai, JCP 43, 3570 (1965).
- (5) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).
- (6) Hooker, Main, JQSRT 8, 1527 (1968); Physica 41, 35 (1969).
- (7) Törring, ZN 23 a, 777 (1968).
- (8) Hildenbrand, Murad, JCP 51, 807 (1969).
- (9) Singh, Upadhyaya, Nair, IJP 43, 665 (1969).
- (10) Czernichowski, Zyrnicki, APP A 37, 865 (1970).
- (11) Nagaraj, Verma, CJP 48, 1436 (1970).
- (12) Raymonda, Muentner, Klempner, JCP 52, 3458 (1970).
- (13) Rusin, VMUK 25, 397, 526 (1970); 27, 196 (1972).
- (14) Cornet, BCSARB (5) 57, 1069 (1971).

- (15) Elander, Lagerqvist, PS 3, 267 (1971).
- (16) Hildenbrand, IJMSIP 7, 255 (1971).
- (17) Bosser, Lebreton, Marsigny, CR C 275, 531 (1972).
- (18) Cornet, Dubois, CJP 50, 630 (1972).
- (19) Hedelund, Lambert, ApL 11, 71 (1972).
- (19a) Heil, Schaefer, JCP 56, 958 (1972).
- (20) Smith, Liszt, JQSRT 12, 505 (1972).
- (21) Liszt, Smith, JQSRT 12, 947 (1972).
- (22) Bredohl, Cornet, Dubois, Remy, CJP 51, 2332 (1973).
- (23) Elander, Smith, ApJ 184, 311 (1973).
- (24) Lagerqvist, Renhorn, Elander, JMS 46, 285 (1973).
- (25) Nagai, Niwa, Shinmei, Yokokawa, JCS FT I 69, 1628 (1973).
- (26) Beer, Lambert, Sneden, PASP 86, 806 (1974).
- (27) Bredohl, Cornet, Dubois, Remy, JP B 7, L66 (1974).
- (28) Davis, Muentner, JCP 61, 2940 (1974).
- (29) Hager, Wilson, Hadley, CPL 27, 439 (1974).
- (30) Hildenbrand, Murad, JCP 61, 1232 (1974).
- (31) Honerjäger, Tischer, ZN 29 a, 1695 (1974).
- (32) Lagerqvist, Renhorn, JMS 49, 157 (1974).
- (33) Lagerqvist, Renhorn, APH 35, 155 (1974).
- (34) Lovas, Krupenie, JPCRD 3, 245 (1974).
- (35) Singh, Bredohl, Remy, Dubois, CJP 52, 569 (1974).
- (36) Barrow, Stone, JP B 8, L13 (1975).
- (37) Bredohl, Cornet, Dubois, JP B 8, L16 (1975).
- (38) Deutsch, Deutsch, Elander, Lagerqvist, PS 12, 248 (1975).
- (39) Hager, Harris, Hadley, JCP 63, 2810 (1975).
- (40) Kaifu, Buhl, Snyder, ApJ 195, 359 (1975).
- (41) Buhl, Snyder, Lovas, Johnson, ApJ 201, L29 (1975).
- (42) Podkorytova, OS(Engl. Transl.) 38, 637 (1975).
- (43) Singh, AA 44, 411 (1975).

(continued p.609)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{28}\text{Si}^{16}\text{O}^+$		$D_0^0 = 4.9_8 \text{ eV}^a$						$B \rightarrow X,^c$ R 26016.55 Z	AUG 1977 (1)*(2)*(5)	
B $2\Sigma^+$				$[0.7103]^b$		$[11.9]$	$[1.527_1]$			
X $2\Sigma^+$	0			$[0.7178]^b$		$[12.0]$	$[1.519_1]$			
$^{28}\text{Si}^{31}\text{P}$		$\mu = 14.6995860$	$D_0^0 = 3.7_3 \text{ eV}^a$							SEP 1977
$^{28}\text{Si}^{32}\text{S}$		$\mu = 14.9206889$	$D_0^0 = 6.4_2 \text{ eV}^a$							AUG 1977 A
E $1\Sigma^+$	41915.8	405.6 Z	1.60^b	0.22137^c	0.00139^d		2.2591	$E \leftrightarrow X,^e$ R 41744.0 Z	(2)*(6)(12)	
I $1\Sigma^-$	$\leq 37462^f$	$\cong 404.9$	1.1_8	$\cong 0.214_2$	0.001_8		$\leq 2.29_7$		(5)	
C 1Δ	37269^f	439.9	3.9_7	0.226_9	0.002_8		2.23_1		(5)	
e $3\Sigma^-$	$\leq 35322^f$	$\cong 407.2$	1.7_7	$\cong 0.223_0$	0.002_9		$\leq 2.25_1$		(5)(3)	
D 1Π	35026.8_6	513.1_2 Z	2.9_3	0.2664_7^{gc}	0.0021_6	2.91^h	2.059_1	$D \leftrightarrow X,$ R 34908.5 ₁ Z	(1)*(3)*(5)	
a $3\Pi_1$	$[30239.2]$	Only $v'=0$ observed		$[0.28180]$			$[2.0023]$	$a \rightarrow X,$ R 29865.0 Z	(14)	
X $1\Sigma^+$	0	749.64 Z	2.577^i	0.30352788^c	0.00147308^j	2.01	1.929321^k	Microwave sp. ^l	(10)(15)	
$^{28}\text{Si}^{(80)}\text{Se}$		$(\mu = 20.7224706)$	$D_0^0 = 5.64 \text{ eV}^a$							AUG 1977
E	38505.9	308.8 H	1.95^b					$E \leftarrow X,$ R 38370.3 H	(2)	
D 1Π	32450.3	399.8 H	1.93					$D \leftrightarrow X,$ R 32360.2 H	(1)*(2)	
a $(3\Pi_1)$	(25077)	$[(412)]$ H						$a \rightarrow X,$ R 24993.7 ₃ H	(5)	
X $1\Sigma^+$	0	580.0 H	1.78	0.1920117^c	0.0007767^c	0.842^c	2.058324	Microwave sp.	(3)	
$^{28}\text{Si}^{(130)}\text{Te}$		$(\mu = 23.0194111)$	$D_0^0 = 4.64 \text{ eV}^a$							AUG 1977
E	33991	242 H	$(3.63)^b$					$E \leftarrow X,$ R 33871 H	(2)	
D 1Π	28661.8	338.6 H	1.70					$D \leftrightarrow X,$ R 28590.4 H	(1)*(2)	
X $1\Sigma^+$	0	481.2 H	1.30							

SiO (continued):

- (44) Bredohl, Remy, Cornet, JP B 2, 2307 (1976).
- (45) Lakshman, Rao, Naidu, Pramāṇa 7, 369 (1976).
- (46) Oddershede, Elander, JCP 65, 3495 (1976).
- (47) Shanker, Linton, Verma, JMS 60, 197 (1976).
- (48) Verma, Shanker, JMS 63, 553 (1976).
- (48a) Renhorn, Dissertation (Stockholm, 1976).
- (49) Field, Lagerqvist, Renhorn, PS 14, 298 (1976);
JCP 66, 868 (1977).
- (50) Manson, Clark, De Lucia, Gordy, PR A 15, 223 (1977).
- (51) Linton, Capelle, JMS 66, 62 (1977).

SiO⁺: ^aD⁰(SiO) + I.P.(Si) - I.P.(SiO).

^bSpin splitting constants $\gamma_0' = -0.0066$, $\gamma_0'' = +0.0028$.

^cThere has been some doubt whether this spectrum is due to SiO⁺ or SiN (2)(3) but the recent work of (5) seems to settle this point in favour of SiO⁺. Another extensive system of R shaded bands, also ascribed to B→X of SiO⁺, has been observed (4) in discharges through O₂ + SiCl₄ and, with much higher intensity, from a hollow cathode containing a stoichiometric mixture of SiO₂ + Si; $\nu_{00} = 30500.1$, $\omega_e' = 634.90$, $\omega_e'x_e' = 4.45$, $B_e' = 0.5180$, $\alpha_e' = 0.0054$, $\omega_e'' = 976.06$, $\omega_e''x_e'' = 5.57$, $B_e'' = 0.6103$, $\alpha_e'' = 0.0051$. No doublet splitting was observed and, as pointed out by (5), the lower state B value does not fit with those of the Rydberg states of SiO.

- (1) Woods, PR 63, 426 (1943).
- (2) Nagaraj, Verma, CJP 46, 1597 (1968).
- (3) Dunn, Rao, Nagaraj, Verma, CJP 47, 2128 (1969).
- (4) Cornet, Dubois, Gerkens, Tripnaux, BSRSL 41, 183 (1972).
- (5) Singh, Bredohl, Remy, Dubois, JP B 6, 2656 (1973).

SiP: ^aThermochemical value (mass-spectrom.)(1).

(1) Smoes, Depière, Drowart, RIHTR 2, 171 (1972).

SiS: ^aFrom a short extrapolation of the vibrational levels of the E state (4) assuming dissociation into ³P₂ + ³P₂ (8).

^b $\omega_e\gamma_e = -0.028$.

^cRKR potential curves (7)(13).

^d $\gamma_e = -0.000018$.

^eBands in the near UV and visible region (3490 - 6170 Å) first described by (1) have been shown (12) to be part of the E→X system ($1 \leq v' \leq 17$, $20 \leq v'' \leq 51$). Franck-Condon factors (13).

^fThe constants for these states have been derived (5) from perturbations in D ¹Π; the vibrational numbering is uncertain except for C ¹Δ.

^gNumerous perturbations due to interactions with e ³Σ⁻, C ¹Δ, and I ¹Σ⁻.

^h $\beta_e = -0.03 \times 10^{-7}$.

ⁱ $\omega_e\gamma_e = +0.00052$.

^j $\gamma_e = -8.6 \times 10^{-8}$.

^kFrom studies of four different isotopes the equilibrium internuclear distance at the minimum of the Born-Oppenheimer potential curve can be derived: $r_e^{(B0)} = 1.929264$ Å (10).

^l $\mu_{e\ell}(v=0) = +1.73$ D (⁺SiS⁻), see (7a)(9)(10); $g_J = -0.09097 - 0.00029(v+\frac{1}{2})$ (11); Si³³S hyperfine structure (9); adiabatic and non-adiabatic corrections (10).

(References on p.611)

SiSe: }
SiTe: } See p.611.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{152})\text{Sm}^{(35)}\text{Cl}$		$(\mu = 28.4258078)$				$D_0^0 \geq 4.3_4 \text{ eV}^a$				SEP 1976 (1)
$\text{Bands in the region } 12500 - 17200 \text{ cm}^{-1} \text{ of the low-resolution Sm + Cl}_2 \text{ chemiluminescence spectrum have been attributed to SmCl.}$										
$(^{152})\text{Sm}^{19}\text{F}$		$(\mu = 16.8866373)$				$D_0^0 = 5.4_6 \text{ eV}^a$				SEP 1976 (2)(3)
$\text{Unresolved emission in the region } 14000 - 33000, \text{ maximum at } 24000 \text{ cm}^{-1}.$										
$(^{152})\text{Sm}^{16}\text{O}$		$(\mu = 14.4713000_4)$				$D_0^0 = 5.90 \text{ eV}^a$	$\text{I.P.} = 5.5_5 \text{ eV}^b$			SEP 1977 (1)(2)* (3) (6)(7)(9)
$\text{Large number of unclassified, mostly R shaded emission bands from } 13200 \text{ to } 23300 \text{ cm}^{-1}.$										
$\text{Low-resolution chemiluminescence spectra have two broad maxima at } 15600 \text{ and } 21100 \text{ cm}^{-1}.$										

SmCl: ^aFrom the Sm + Cl $_2$ chemiluminescence spectrum (1).

(1) Yokozeki, Menzinger, CP 14, 427 (1976).

SmF: ^aThermochemical value (mass-spectrom.)(1); consistent with lower limits from the Sm + F $_2$ chemiluminescence spectrum (2)(3).

(1) Zmbov, Margrave, JINC 29, 59 (1967).

(2) Dickson, Zare, CP 7, 361 (1975).

(3) See ref. (1) of SmCl.

SmO: ^aThermochemical value (mass-spectrom.)(10), compatible with (7) and superseding earlier results of (4)(5).

^bCorrected electron impact appearance potential (8).

(1) Piccardi, AANL 21, 589 (1935); 25, 86 (1937).

(2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(3) Herrmann, Alkemade, "Chemical Analysis by Flame Photometry", 2nd rev. ed., Interscience (1963).

(4) Ames, Walsh, White, JPC 71, 2707 (1967).

(5) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

(6) Edelstein, Eckstrom, Perry, Benson, JCP 61, 4932 (1974).

(7) See ref. (2) of SmF.

(8) Ackermann, Rauh, Thorn, JCP 65, 1027 (1976).

(9) See ref. (1) of SmCl.

(10) Hildenbrand, CPL 48, 340 (1977).

SiS (continued):

- (1) Barrow, Jevons, PRS A 169, 45 (1938).
- (2) Vago, Barrow, PPS 58, 538 (1946).
- (3) Lagerqvist, Nilheden, Barrow, PPS A 65, 419 (1952).
- (4) Robinson, Barrow, PPS A 67, 95 (1954).
- (5) Nilheden, AF 10, 19 (1955).
- (6) Barrow, Deutsch, Lagerqvist, Westerlund, PPS 78, 1307 (1961).
- (7) Nair, Singh, Rai, JCP 43, 3570 (1965).
- (7a) Murty, Curl, JMS 30, 102 (1969).
- (8) Barrow, DONNSPEC (1970), p. 323.
- (9) Hoeft, Lovas, Tiemann, Törring, ZN 24 a, 1422 (1969); JCP 53, 2736 (1970).
- (10) Tiemann, Renwanz, Hoeft, Törring, ZN 27 a, 1566 (1972).
- (11) Honerjäger, Tischer, ZN 28 a, 1374 (1973).
- (12) Bredohl, Cornet, Dubois, Wildéria, JP B 8, L259 (1975).
- (13) Katti, Korwar, APH 39, 145 (1975).
- (14) Bredohl, Cornet, Dubois, JP B 9, L207 (1976).
- (15) Tiemann, JPCRD 5, 1147 (1976).

- SiSe: ^aFrom an extrapolation of the vibrational levels of the E ¹ Σ^+ state assuming dissociation into ³P₂ + ³P₂ (2)(4).
^b_wy_e = -0.032.
^cRotational constants for ²⁸Si⁸⁰Se; (3) gives constants for eight isotopic species.
- (1) Barrow, PPS 51, 267 (1939).
 - (2) See ref. (2) of SiS.
 - (3) Hoeft, ZN 20 a, 1122 (1965).
 - (4) See ref. (8) of SiS.
 - (5) Lebreton, Bosser, Ferran, Marsigny, JP B 8, L141 (1975).
- SiTe: ^aAverage of two recent thermochemical determinations (3)(4), corrected for the new value of D₀⁰(Te₂); see also (5).
^b_wy_e = (+0.13).
- (1) See ref. (1) of SiSe.
 - (2) See ref. (2) of SiS.
 - (3) Exsteen, Drowart, Auwera-Mahieu, Callaerts, JPC 71, 4130 (1967).
 - (4) Brebrick, JCP 49, 2584 (1968).
 - (5) Barrow, DONNSPEC (1970), p. 323 and 367.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(118,120)Sn ₂										SEP 1977 A
(120)Sn(79)Br										SEP 1977
$(\mu = 47.593081_9)$ Unidentified absorption bands in the region 42300 - 45800 cm^{-1} .										(6)
E	(43570)	[320]						E \leftarrow X ₁ ,	43607	(6)
D	(42742)	[269]						D \leftarrow X ₁ ,	42753	(6)
C	[40869]							C \leftarrow X ₁ ,	40746	(6)
B (² Σ)	33062.3	304.3	H	0.7 ₁	No emission from $v' \geq 1$.			B \rightarrow X ₂ , V	(30628) ^a	(1)* (4)
								B \leftrightarrow X ₁ ,	33090.8	H
A (² Δ)	(27063) 26695	[163.6] 169.1	H	6.8				A \rightarrow X, R	24557.9 26654.3	H (1)*
A' (² Σ)	(18717) ^b	164.1	H	0.9				A' \rightarrow X ^c , R	18675.8	H (2)* (3)
X ₂ ² $\Pi_{3/2}$	(2463)	247.2 ^d	H	0.6 ₃ ^d						
X ₁ ² $\Pi_{1/2}$	0									
¹²⁰ Sn ³⁵ Cl										SEP 1977
$\mu = 27.0731195$ Several weak diffuse absorption bands, 45400 - 47600 cm^{-1} . Strong absorption continua 29000 - 33000 and 40000 - 53000 cm^{-1} [see, however, (7)].										(8) (3)
C	(43718) 43650	399.3 ^a	H	1.1				C \leftarrow X, ^b V	41384 ^a 43674 ^a	H (3)(8)
C'	41229	419.3 ^a	H	1.7				C' \leftarrow X ₁ , ^b V	41263 ^a	H (8)
B ² Σ^+	33583.3	431.8	H ^Q	1.25	0.1216	0.0006	2.263	B \leftrightarrow X, V	31265.4 33623.6	H ^Q (1)* (3)(4) (8)(9)(12) (14)
A c	28963 28692	303.3 ^a 300.8 ^a	H ^Q	3.7 4.0	c			A \leftrightarrow X, R	26580 ^a 28666 ^a	H ^Q (1)* (2)(3) (4)
A' ² Σ^+	19418.4	232.3	H	0.71	[0.0908]		[2.619]	A' \rightarrow X ₁ , R	19359.1	H (4)* (5)(6) (10)(12)
X ₂ ² $\Pi_{3/2}$	2356.6	354.4	H ^Q	1.05	0.1122	0.0004	2.356			
X ₁ ² $\Pi_{1/2}$	0	351.1	H ^Q	1.06	0.1117 ^d	0.0004	2.361			

Sn₂: ^aThermochemical value (mass-spectrom.) (1)(2).

- (1) Drowart, Honig, JPC 61, 980 (1957).
- (2) Ackerman, Drowart, Stafford, Verhaegen, JCP 36, 1557 (1962).

SnBr: ^a0-0 head obscured by an atomic line; the v" numbering of this subsystem is uncertain.

^bAssuming X₁ as the lower state of the A'→X bands; see ^c.

^cIt is not clear whether the lower-state component is X₁ or X₂. (5) suggest X₁ and assign a number of weaker bands near 6300 Å to A'→X₂.

^dAverage of the constants obtained by (1)(4).

- (1) Jevons, Bashford, PPS 49, 554 (1937).
- (2) Sarma, Venkateswarlu, JMS 17, 203 (1965).
- (3) Naegeli, Palmer, JMS 21, 325 (1966).
- (4) Oldershaw, Robinson, TFS 64, 616 (1968).
- (5) Chatalic, Deschamps, Pannetier, CR C 269, 584 (1969).
- (6) Oldershaw, Robinson, TFS 67, 2499 (1971).

SnCl: ^aNatural Sn isotopic mixture.

^bAccording to (13) also observed in emission.

^cOriginally assumed to be ²Δ, this state has recently been reinterpreted as ⁴Σ⁻ (Ω=1/2 and 3/2) on the basis of a tentative analysis of incompletely resolved rotational structure (11).

^dΛ-type doubling Δv_{fe} = -0.009(J+½) (12).

- (1) Jevons, PRS A 110, 365 (1926).
- (2) Ferguson, PR 32, 607 (1928).
- (3) Fowler, PR 62, 141 (1942).
- (4) Sarma, Venkateswarlu, JMS 17, 252 (1965).
- (5) See ref. (3) of SnBr.
- (6) Pannetier, Deschamps, JCPPB 65, 1164 (1968).
- (7) Hastie, Hauge, Margrave, JMS 29, 152 (1969).
- (8) Oldershaw, Robinson, JMS 32, 469 (1969).
- (9) Richter, ZPC (Frankfurt a.M.) 71, 303 (1970).
- (10) Chatalic, Iacocca, Pannetier, JCPPB 69, 82 (1972).
- (11) Chatalic, Iacocca, Pannetier, JCPPB 70, 481 (1973).
- (12) Chatalic, Iacocca, Pannetier, JCPPB 70, 908 (1973).
- (13) Katti, Korwar, PL A 48, 461 (1974); CS 43, 374 (1974).
- (14) Katti, Korwar, IJPAP 13, 710 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{118}\text{Sn}^{19}\text{F}$		$\mu = 16.3618865$ $D_0^0 = 4.9_0 \text{ eV}^a$ Strong absorption continua with maxima at 41000 and 53000 cm^{-1} .								SEP 1977	
G $^2\Delta$	(46427) (46338)	[609.9] ^b	H		[0.2870] ^c		[0.22 ₅] ^c	[1.895]	G \leftrightarrow X, V	44121.9 Z 46351.8 ^b H	(1)(3)
F ($^2\Sigma$)	45500.5	688.2 ^d	H	4.6 ₅					F \rightarrow A, V	25497.0	(3)
									F \leftrightarrow X, V	43233.1 45552.6 ^d H	(1)(3)
E	42137.1 41856.1	677.0 ^d	H	3.0					E \leftrightarrow X, V	39864.5 ^d H 41903.0 ^d H	(1)(3)
D	(41341)	[622] ^d	H						D \rightarrow X, V	39041.9 41361.4 ^d H	(3)
C $^2\Delta$	40831 40760	[600] ^d	H	(5.4)	[0.2856] ^c		[0.22 ₃] ^c	[1.899]	C \leftrightarrow X, V	38524.7 Z 40772.8 ^d H	(1)(3)(6)
B $^2\Sigma^+$	34109.0	677.6 ^d	H	2.74	[0.2896]		[0.24 ₆]	[1.886]	B \rightarrow A, V	14100.9	(3)
									B \leftrightarrow X, V	31836.97 Z (34156.09)	(1)* (4)
B* ($^4\Sigma^-$) ^e									B* \rightarrow X,	33039.8 ^d H	(3)
A $^2\Sigma^+$	20136.9	[415.76]	Z	2.20 ₆	0.2471 ^f	0.0026	[0.38 ₂] ^g	2.042	A \rightarrow X, ^h R	17736.08 Z 20055.58 Z	(2)* (4)(9)*
X $^2\Pi_{3/2}$	2316.9	[582.67]	Z	2.82	0.2738	0.0014	[0.22 ₅] ⁱ	1.940			
X $^2\Pi_{1/2}$	0	[577.64]	Z	2.69	0.2727 ^{jk}	0.0014	[0.26 ₂] ^l	1.944			
$^{120}\text{Sn}^1\text{H}$		$(\mu = 0.99942466)$ $D_0^0 \leq 2.73 \text{ eV}^a$								AUG 1977	
A $^2\Delta$	b				[4.904] ^{cd}		[433] ^e	[1.854 ₆]	A \leftrightarrow X, R	23468.27 Z	(1)(4)*
a $^4\Sigma^-$					[5.3723] ^f		[298] ^g	[1.7719]	a \leftrightarrow X, ^h R	15439.27 Z	(2)(4)*
X $^2\Pi_r$	0 ⁱ				[5.31488] ^j		[207.5]	[1.78146]			
$^{120}\text{Sn}^2\text{H}$		$(\mu = 1.98082851)$								AUG 1977	
A $^2\Delta$	(23790) ^k	[(736)]			[2.5161] ^c	(0.2)	[110.4] ^l	[1.8391]	A \leftarrow X, R	23563.65 Z	(4)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(120) Sn^2H (continued)										
a $^4\Sigma^-$	(15580)	[992.5]	Z	[2.740] ^m	0.13	[80] ⁿ	[1.762]	a ← X,	R 15482.5	Z (4)
X $^2\Pi_r$	0 ^o	[1188.0]	Z	[2.6950] ^p	0.049 ₀	[53.4]	[1.7770]			

SnF: ^aThermochemical value (mass-spectrom.)(7), recalculated

with $D_0^0(\text{CaF}) = 5.4_8 \text{ eV}$.

^bFrom (3) (natural isotopic mixture); (1) give $\Delta G(\frac{1}{2}) = 607$ and 598 cm^{-1} .

^cOnly the $^2\Delta_{5/2}$ component has been analyzed (10).

^dNatural isotopic mixture.

^eAssignment by analogy with GeF (11).

^fSpin doubling constant $\gamma = -0.0836$.

^g $D_1 = 0.32_2 \times 10^{-6}$.

^hFranck-Condon factors (8).

ⁱ $D_1 = 0.25_2 \times 10^{-6}$.

^j Λ -type doubling $\Delta v_{fe} = -0.058_8(J + \frac{1}{2})$.

^kRKR potential curve (5).

^l $D_1 = 0.33_6 \times 10^{-6}$.

(1) Jenkins, Rochester, PR 52, 1135 (1937).

(2) Yuasa, PPMSJ 21, 498 (1939).

(3) Barrow, Butler, Johns, Powell, PPS 73, 317 (1959).

(4) Barrow, Kopp, Merer, PPS 72, 749 (1962).

(5) Singh, Rai, IJPAP 4, 102 (1966).

(6) Uzikov, Kuzyakov, VMUK 23(5), 33 (1968).

(7) Zmbrov, Hastie, Margrave, TFS 64, 861 (1968).

(8) Singh, Dube, IJPAP 2, 164 (1971).

(9) Rai, Singh, SpL 5, 155 (1972).

(10) Ram, Upadhyaya, Rai, JP B 6, L372 (1973).

(11) Merer, private communication.

Sn^1H , Sn^2H :

^aFrom the predissociation in $A^2\Delta$ assuming dissociation into $^3P_2 + ^2S$.

^bSpin coupling constants for $v=0$: $A = 20.41$, $A_J = 0.0625$, $\gamma = 1.23$ (4). For a more elaborate evaluation of these constants (including centrifugal distortion) see (8).

^cRotational constants of (4) based on a modified Hill-Van Vleck expression; see also (8). A case "c" treatment of the same data is given by (11).

^dBroadening of absorption lines above $N' \approx 14$ (4), sharp cut-off in emission at $N' = 17$ (1).

^e $H_0 = -2.3 \times 10^{-7}$; see ^c.

^fSpin splitting constants for $v=0$: $\lambda = 45.78$, $\gamma_1 = 0.190$, $\gamma_2 = 0.191$. ΔB (difference in B values between the states $\Omega = 1/2$ and $3/2$) = -0.0266 . All constants derived by (4) according to the modified expressions [see (4)] for the energy levels of a $^4\Sigma$ state (3). For further refinements see (7)(9). The case "c" treatment of the same data by (11) gives $B_0 = 5.404$ and 5.339 for $\Omega = 1/2$ and $3/2$, respectively. For a discussion of $^4\Sigma_1^-$ in terms of case "a" coupling conditions see (6).

^g $H_0 = -3.3 \times 10^{-8}$.

^hRotational intensity distribution (5)(6).

ⁱ $A_0 = +2178.88 + 0.01719 J(J+1)$ (4); see, however, (8).

(continued p. 617)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(^{120}\text{Sn}^{127}\text{I})$		$(\mu = 61.652004_6)$ Fragments of several overlapping systems of absorption bands in the region $38800 - 46300 \text{ cm}^{-1}$.								SEP 1977 (3)(4)
B ($^2\Sigma$)	32172.8	241.1	H 0.1 ₇					B \leftarrow X, V	32193.9 H	(1)*
A ($^2\Sigma$)	17916.7	129.8	H 0.4 ₆					A \rightarrow X, R	17880.8 H	(2)
X ($^2\Pi_{\frac{1}{2}}$)	0	199.0 ^a	H 0.5 ₅							
$^{120}\text{Sn}^{160}$		$\mu = 14.1123342_7$ $D_0^0 = 5.49 \text{ eV}^a$ Unidentified absorption bands, $64920 - 68360 \text{ cm}^{-1}$. 724 H 21 [466] H Unidentified absorption bands, $53250 - 57670 \text{ cm}^{-1}$. Absorption continuum between 51630 and 51920 cm^{-1} . 508.0 H 2.9 ^c [573.6] Z 3.08 ^d H 0.3145 ₅ ^{ef} 0.0025 4.0 1.948 ₇ A large number of emission bands in the visible and near UV region has been observed by various methods (1)(10)(12). A satisfactory interpretation is still lacking.								SEP 1977 (5) (5)* (5)* (5) (5) (2)(4)* (1)* (3)(6)*
G	58806 ^b	724	H 21					G \leftarrow X, R	58752 H	(5)*
F	(57669)	[466]	H					F \leftarrow X, R	57492 H	(5)*
E	36295	508.0	H 2.9 ^c					E \leftrightarrow X, R	36138 H	(2)(4)*
D $^1\Pi$	29624	[573.6]	Z 3.08 ^d H	0.3145 ₅ ^{ef}	0.0025	4.0	1.948 ₇	D \leftrightarrow X, ^{gh} R	29503.2 Z	(1)* (3)(6)*
B (1)	(24890)	[560]		$B_1 = 0.3010^i$			[1.992]	B \leftarrow X, R	24760	(7)
A (0^+)	(24333)	[555]		[0.2964]			[2.008]	A \leftarrow X, R	24200	(7)
X $^1\Sigma^+$	0	[814.6]	Z 3.73 H	0.3557191 ^f	0.002142 ₉ ^j	(2.66)	1.832505	IR spectrum ^k Microwave sp. ^l		(14) (11)

SnI: ^aFrom the absorption spectrum (1). From the emission spectrum (2) obtain $w_e = 201.6$, $w_e x_e = 0.53$.

(1) Oldershaw, Robinson, TFS 64, 616 (1968).

SnI (continued):

(2) Murty, Haranath, Rao, IJP 45, 203 (1971).

(3) Iacocca, Chatalic, Pannetier, CR C 274, 1892 (1972).

(4) Oldershaw, Robinson, JMS 45, 489 (1973).

SnO: ^aThermochemical value (8). Extrapolation of the E-X v''=0 progression gives a dissociation limit at 45770 cm⁻¹ (5); if it corresponds to ³P₁ + ³P₁ [see (15)] a dissociation energy of 5.45 eV would follow.

^b(5) give 58809.6 which does not fit with their observed (or calculated) v₀₀.

^c-5 x 10⁻⁵(v+ $\frac{1}{2}$)⁵ (valid for v' ≤ 17).

^dw_ey_e = -0.135.

^eSmall Λ-type doubling. Several perturbations, probably by a ¹Π (or ¹Δ) state (6).

^fRKR potential functions (9).

^gFranck-Condon factors, relative band intensities, variation of electronic transition moment with r (16).

^hThe observed ¹¹⁸Sn and ¹¹⁶Sn isotope shifts for the 0-1 band (6) seem to confirm the v' numbering. See, however, (12) who suggest that v' be increased by 1.

ⁱBoth v=1 and v=2 are extensively perturbed.

^jγ_e ≈ -7 x 10⁻⁷.

^kIn argon and nitrogen matrices.

^l(11) gives rotational constants for seven isotopes. Dipole moment from Stark effect of rotation spectrum

SnO (continued):

- μ_{el}(v=0) = 4.3₂ D (13). Zeeman effect (17), g_J(v=0) = -0.1463.
- (1) Mahanti, ZP 68, 114 (1931).
 - (2) Loomis, Watson, PR 45, 805 (1934).
 - (3) Jevons, PPS 50, 910 (1938).
 - (4) Eisler, Barrow, PPS A 62, 740 (1949).
 - (5) Barrow, Rowlinson, PRS A 224, 374 (1954).
 - (6) Lagerqvist, Nilsson, Wigartz, AF 15, 521 (1959).
 - (7) Deutsch, Barrow, Nature 201, 815 (1964).
 - (8) Colin, Drowart, Verhaegen, TFS 61, 1364 (1965).
 - (9) Nair, Singh, Rai, JCP 43, 3570 (1965).
 - (10) Joshi, Yamdagni, IJP 41, 275 (1967).
 - (11) Törring, ZN 22 a, 1234 (1967).
 - (12) Smith, Meyer, JMS 27, 304 (1968).
 - (13) Hoeft, Lovas, Tiemann, Tischer, Törring, ZN 24 a, 1222 (1969).
 - (14) Ogden, Ricks, JCP 53, 896 (1970).
 - (15) Barrow, DONNSPEC (1970), p. 323.
 - (16) Dube, Rai, JP B 4, 579 (1971).
 - (17) Honerjäger, Tischer, ZN 28 a, 1372 (1973).

Sn¹H, Sn²H (continued):

- ^jΛ-type doubling in ²Π_{1/2}(v=0), Δv_{fe} = +1.003(J+ $\frac{1}{2}$) - 1.76 x 10⁻⁴(J+ $\frac{1}{2}$)³ (4).
- ^kSpin coupling constants for v=0: A = 8.52, A_J = 0.0225, γ = 0.555. The large difference from Sn¹H remains unexplained; see (10)(11).
- ^lH₀ = -0.135 x 10⁻⁷; see ^c. | explained; see (10)(11).
- ^mSpin splitting constants for v=0: λ = 45.0, γ₁ = 0.076, η_{H0} = -0.13 x 10⁻⁸. | γ₂ = 0.0883. ΔB(see ^f) = -0.012.
- ^oA₀ = 2177.05 + 0.0080 J(J+1).
- ^pΔv_{fe}(²Π_{1/2}, v=0) = +0.5076(J+ $\frac{1}{2}$) - 0.000045(J+ $\frac{1}{2}$)³.

- (1) Watson, Simon, PR 55, 358 (1939).
- (2) Watson, Simon, PR 57, 708 (1940).
- (3) Hougen, CJP 40, 598 (1962).
- (4) Klynning, Lindgren, Åslund, AF 30, 141 (1965).
- (5) Klynning, AF 31, 281 (1966).
- (6) Kopp, Hougen, CJP 45, 2581 (1967).
- (7) Kovács, Korwar, JP B 4, 759 (1971).
- (8) Kovács, Vujisić, JP B 4, 1123 (1971).
- (9) Kovács, Pacher, JP B 4, 1633 (1971).
- (10) Veseth, Physica 56, 286 (1971).
- (11) Veseth, JMS 48, 283 (1973).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-8}cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$^{120}\text{Sn}^{32}\text{S}$										AUG 1977
$\mu = 25.2414174$ $D_0^0 = 4.77 \text{ eV}^a$										
Continuous absorption from 56470 to 56887 cm^{-1} .										(2)
G^b	[56171]	$v=0$ only.						$G \leftarrow X$, R	55928 H	(2)
F^b	(52257)	(408) H	(4.5)					$F \leftarrow X$, R	52217 H	(2)
E	$^1\Sigma^+$ 33037.0	294.25 H	1.15	$B_{20} = 0.0889$ $B_{19} = 0.0915$				$E \leftrightarrow X$, R	32941 H	(1)* (2)(3)
D	$^1\Pi$ 28336.6 ₀	331.35 Z	1.265	0.12023 ^{cd}	0.00070		2.3569	$D \leftrightarrow X$, R	28258.67 Z	(1)* (3)
The spectrum in the visible and near UV region is very complex, both in absorption and in emission (1)(3)(7); partial analysis by (3):										
C'	1 [23950.3]	Only one level ^e analyzed.		[0.1075]			[2.493]	$C' \leftrightarrow X$, R	23707.0 Z	(3)
B	1 (23589.8)	$[366.60]^f$ Z		[0.1214]	g		[2.345]	$B \leftrightarrow X$, R	23529.82 Z	(3)
A	0^+ [22915.97]	Only one level ^h analyzed.		[0.1184]			[2.375]	$A \leftrightarrow X$, R	22672.68 Z	(3)
a		Fluorescence bands in rare gas matrices, 18300-14300 cm^{-1} .						$a \rightarrow X$,	(18300)	(8)
X	$^1\Sigma^+$ 0	487.26 Z	1.358	0.13686139 ^d	0.00050563 ⁱ	4.24	2.209026	IR spectrum ^j		(12)
								Microwave sp. ^k		(9)
$(^{120}\text{Sn}^{80})\text{Se}$										AUG 1977
$(\mu = 47.954301_7)$ $D_0^0 = 4.2_0 \text{ eV}^a$										
F	(47850)	(290)						$F \leftarrow X$, R	(47830) H	(3)*
E	30738.9	196.6 H	0.77 ^b					$E \leftrightarrow X$, R	30671.6 H	(2)(3)*
D	27549.6	225.1 H	0.69					$D \leftrightarrow X$, R	27496.6 H	(1)(2)* (3)*
A definitive analysis of the visible absorption bands (15800-23800 cm^{-1}) is still lacking.										
At least three or four systems seem to be present with upper state frequencies of ~ 226 and 218 cm^{-1} , but there is considerable disagreement concerning the assignments of the bands.										(1)(7)(8)
X	$^1\Sigma^+$ 0	331.2 H	0.736	0.0649977 ^c	0.0001704 ^d	1.1	2.325601	IR spectrum ^e		(9)
								Microwave sp. ^f		(5)

SnS: ^aThermochemical value (4); agrees fairly well with values derived from the continuous absorption ($D_0^0 \leq 4.84$ eV) and from a short extrapolation of the vibrational levels of the E state ($D_0^0 = 4.81$ eV) if dissociation into $^1D + ^1D$ and $^3P_1 + ^3P_1$, respectively, is assumed.

^b_p and _q of (2).

^cPerturbations.

^dRKR potential functions (6).

^eCalled *z* by (3) and renamed *C'* by (5); *v* numbering uncertain. Low *J* lines (*J* < 29) are weak or absent causing the headless appearance of the bands.

^fThe two levels *x* and *w* of (3) are believed (5) to belong to the same electronic state; *v* numbering uncertain. Rotational perturbations in both observed levels.

^g $B_1 = 0.1218$; see ^f.

^hCalled *y* by (3), renamed *A* by (5); *v* numbering uncertain.

ⁱ $-1.87 \times 10^{-7}(v+\frac{1}{2})^2 - 4 \times 10^{-9}(v+\frac{1}{2})^3$.

^jIn argon matrix.

^k $\mu_{el} = 3.17 + 0.022(v+\frac{1}{2})$ D (9)(11); see also (10). ^{33}S hf structure (11).

(1) Rochester, PRS A 150, 668 (1935).

(2) Barrow, Drummond, Rowlinson, PPS A 66, 885 (1953).

(3) Douglas, Howe, Morton, JMS 7, 161 (1961).

(4) Colin, Drowart, JCP 37, 1120 (1962).

(5) Barrow, Fry, Le Bargy, PPS 81, 697 (1963).

(6) Nair, Singh, Rai, JCP 43, 3570 (1965).

(7) Yamdagni, Joshi, IJP 40, 495 (1966).

(8) Smith, Meyer, JMS 27, 304 (1968).

(9) Hoeft, Lovas, Tiemann, Törring, ZN 24 a, 1222 (1969).

SnS (continued):

- (10) Murty, Curl, JMS 30, 102 (1969).
- (11) Hoeft, Lovas, Tiemann, Törring, JCP 53, 2736 (1970).
- (12) Marino, Guerin, Nixon, JMS 51, 160 (1974).

SnSe: ^aFrom thermochemical data (mass-spectrom.)(4), recalculated with $D_0^0(\text{Se}_2) = 3.411$ eV (see ^a of Se_2). Assuming dissociation into $^3P_1 + ^3P_1$ at the dissociation limit of the E state [see ^b and (7)] gives $D_0^0 = 4.08$ eV.

^b $\omega_{ey_e} = -0.0016$. Vibrational levels observed to *v*=29; a short extrapolation yields a dissociation limit at 35470 cm^{-1} while the banded absorption seems to go over into a continuum at 36570 cm^{-1} .

^cRotational constants for $^{120}\text{Sn}^{80}\text{Se}$; see (5) who gives similar data for 28 other isotopic molecules.

^d $\mu_{el} = -1.3 \times 10^{-7}$.

^eIn argon matrix.

^f $\mu_{el}(v=0) = 2.82$ D, from Stark effect of microwave sp. (6).

(1) Walker, Straley, Smith, PR 53, 140 (1938).

(2) Barrow, Vago, PPS 55, 326 (1943).

(3) Vago, Barrow, PPS 58, 707 (1946).

(4) Colin, Drowart, TFS 60, 673 (1964).

(5) Hoeft, ZN 21 a, 437 (1966).

(6) Hoeft, Lovas, Tiemann, Törring, ZN 24 a, 1843 (1969).

(7) Barrow, DONNSPEC (1970), p. 376/7.

(8) Yamdagni, JMS 33, 531 (1970).

(9) See ref. (12) of SnS.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
(120)Sn(130)Te											
		$(\mu = 62.351952_6) \quad D_0^0 = 3.69 \text{ eV}^a$								AUG 1977	
J	(47260)	(230)	H					J \leftarrow X, R	(47245)	H (4)(5)*	
I	44033.5	229.7	H	1.25 ^b				I \leftarrow X, R	44018.4	H (4)(5)*	
H	30818.3	201.0	H	0.6				H \leftarrow X, R	30789.0	H (3)(4)	
G	29071.8	200.8	H	0.3				G \leftarrow X, R	29042.5	H (3)(4)	
F	28545.9	98.0	H	1.0				F \leftarrow X, R	28465.0	H (3)(4)	
E	(27642.8)	(135.0)	H	(2.5)				E \leftrightarrow X, ^c R	(27580.0)	H (1)(3)(5)*	
D	25444.3	179.1	H	0.40				D \leftrightarrow X, R	25404.1	H (1)*(2)*(5)*	
C	21418.6	218.1	H	0.98				C \leftarrow X, R	21397.8	H (2)*	
B	20394.9	230.3	H	1.53 ^d				B \leftarrow X, R	20380.0	H (2)*	
A	16844.0	178.5	H	0.44				A \leftarrow X, R	16803.5	H (2)*	
X	¹ Σ^+ 0	259.5	H	0.50	0.04247917 ^e	0.00009543 ^f	0.0055	2.522814	Microwave sp. ^g	(7)	
³²S¹⁶O											
		$\mu = 10.6613029_2 \quad D_0^0 = 5.359 \text{ eV}^a \quad \text{I.P.} = 10.29 \text{ eV}^b$								AUG 1977	
		Potential energy diagram (17).									
		Fragment of another system near 70700 cm^{-1} .								(24)	
E (³ Π)	(67884)	[1220]						E \leftarrow X, {	{ 68092 67921 67746	(18)	
D (³ Π)	(54340)	[1254]						D \leftarrow X, {	{ 54586 54394 54259	(18)	
C	(42200)	(170)	{ State causing perturbations and predissociations in B ³ Σ^- .				(2.2)			(17)	
B	³ Σ^- 41629	630.4 ^{cd}	H	4.79 ^c	0.502 ₀ ^{ef}	0.006 ₂	(1.28)	1.775	B ^g \leftrightarrow X, ^h R	41370	(1)(2)(2a) (17)*
A	³ Π { 2 38622 1 38462 0 38306	412.7 ⁱ	Z	1.7	0.6164	0.0204 ^j	(4.8)	1.601 ₆	A ⁿ \leftrightarrow X, R {	38255 ^k	(17)*
		413.3 ⁱ	Z	1.6	0.6107 ^l	0.0194 ^m	(4.0)	1.609 ₁		38095 ^k	
		415.2 ⁱ	Z	1.6	0.6067 ^o	0.0194 ^m	(3.7)	1.614 ₄		37940 ^k	

SnTe: ^aThermochemical value (mass-spectrom.)(6), corrected for ^b $w_e y_e = -0.003$. | the new value of $D_0^0(\text{Te}_2)$.

^cAccording to (5) the assignments in this system are quite uncertain; (5) give $v_e \approx 28000$, $w_e' \approx 150$.

^d $w_e y_e = -0.013$.

^eRotational constants for $^{120}\text{Sn}^{130}\text{Te}$.

^f $-5.3 \times 10^{-8}(v+\frac{1}{2})^2 + 1.8 \times 10^{-9}(v+\frac{1}{2})^3$.

^gDipole moment of $^{120}\text{Sn}^{130}\text{Te}$: $\mu_{el}(v=0) = 2.19$ D, from Stark effect of microwave spectrum (8). Microwave spectra have been observed for 27 isotopic molecules (7).

(1) Barrow, PPS 52, 380 (1940).

(2) Barrow, Vago, PPS 56, 78 (1944).

(3) Sharma, PNASI A 14, 232 (1945).

(4) Sharma, Nature 157, 663 (1946).

(5) Vago, Barrow, PPS 58, 707 (1946).

(6) Colin, Drowart, TFS 60, 673 (1964).

(7) Hoeft, Tiemann, ZN 23 a, 1034 (1968).

(8) Hoeft, Lovas, Tiemann, Törring, ZN 24 a, 1843 (1969).

SO: ^aFrom the first predissociation limit in B $^3\Sigma^-$ (see ^e) assuming that it corresponds to dissociation into $^3P_2 + ^3P_2$. A similar value ($D_0^0 = 5.36_4$ eV) follows from the assumption that the convergence limit of the B state (see ^d) corresponds to $S(^1D) + O(^3P_2)$. The value given here has been confirmed by thermochemical measurements ^bFrom the photoelectron spectrum (25)(29). | (5); s. also (16). ^cThe constants given represent the best approximation for $v \leq 6$ (2). ^dVibrational levels observed to $v'=30$, very close to the convergence limit $S(^1D) + O(^3P)$ at 52500 ± 100 cm^{-1} (2a) (17). A large drop in the value of ΔG occurs near $v=16$ owing to an avoided crossing with another $^3\Sigma^-$ state (3)

SO (continued):

(17). Lower vibrational levels appear to converge to a limit at ~ 59090 cm^{-1} corresponding to $S(^3P) + O(^1D)$.

^eStrong rotational perturbations, particularly for $v=1$ and 2 (1)(4)(20) and $v=7, 11$ (17). Predissociation (breaking-off in emission) for $v=0, 1, 2, 3$ above $N=66, 53, 39, 6$, respectively (1), leading to a dissociation limit near 43224 cm^{-1} . A second predissociation (diffuseness in absorption) sets in above $v=8$ and reaches its maximum for $v=14, 15$, substantially above the corresponding dissociation limit $^3P + ^3P$ (17).

^fSpin splitting constants $\lambda_0 = 3.5$, $\gamma_0 = 0.010$ or -0.020 (6).

^gRadiative lifetimes $\tau = 17.3, 16.6, 16.2$ ns for $v=0, 1, 2$, respectively (19).

^hFranck-Condon factors (26)(30); measured relative intensities, variation of electronic transition moment with r (30).

ⁱConstants derived from $v=1\dots 4$; $v=0$ is perturbed. $\Delta G(\frac{1}{2}) = 425, 416, 414$ for $^3\Pi_0, ^3\Pi_1, ^3\Pi_2$, respectively. ΔG decreases rapidly above $v=4$.

^j $\gamma_e = +0.0010$.

^kApproximate origins for the deperturbed 0-0 band, by extrapolation from the unperturbed levels $v=1\dots 4$; see ⁱ.

^l Λ -type doubling $\Delta v_{fe} = +0.00031 J(J+1)$.

^m $\gamma_e = +0.0009$.

ⁿRadiative lifetime $\tau = 12.4$ ns corresponding to a band oscillator strength $f \approx 0.018$ near the Franck-Condon maximum (2-0 band); see (27).

^o Λ -type doubling $\Delta v_{fe} \approx +1.2$ cm^{-1} , slightly dependent on J .

(continued p. 622)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-6}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{32}\text{S}^{16}\text{O}$ (continued)										
b $1\Sigma^+$ a 1Δ	10510.0 (6350) ^r	1068.6 ₆ ^p Z	7.2 ₅	0.7026 ₂ [0.7103383] ^s	0.0063 ₅	[1.20] ^q [1.168]	1.5001 [1.491971]	b→X, R 10469.33 Z Microwave sp. ^t ESR sp. ^u IR sp. ^w Microwave sp. ^x ESR sp.	(15)* (22)* (21)(39) (8)(26a)(27a) (35) (6)(7)(10) (31)(32)(39) (9)(12)(34)	
X $3\Sigma^-$	0	1149.2 ₂ ^p Z	5.6 ₃	0.7208171 ^v	0.005736 ₇	[1.134]	1.481087			
$^{32}\text{S}^{16}\text{O}^+$										
				$D_0^0 = 5.43 \text{ eV}^a$						AUG 1977
C (2Π) B ($2\Sigma^-$) b $4\Sigma^-$	(77100) 49780 37690	1000 990	All data obtained from the photoelectron spectrum of SO (1); bond lengths derived from Franck-Condon analyses of the observed spectra.				(1.55) (1.53 ₅)			
A (2Π) a 4Π	(35600) (26170)	800					(1.64)			
X $2\Pi_r$	340 0	1360					(1.42 ₄)			

SO (continued):

^pVibrational constants of (22); the older values of (2) (15) are based on an extrapolation of the ground state vibrational levels (1) required by the revised v'' numbering of (2). This change has been confirmed by isotope studies (14). IR fundamental in Ar matrix: $\Delta G(\frac{1}{2}) = 1136.7$ cm^{-1} . $qD_1 = 1.30 \times 10^{-6}$. (35).

^rFrom a comparison with O_2 and S_2 (15).

^s"True" B_0 of (39); the effective value is 0.7103476.

^t $\mu_{\text{el}} = 1.32 \text{ D}$ [average of values obtained from Stark effect

SO (continued):

of ESR (11)(23) and microwave (21) spectra].

^uThe ^{33}S hf interaction has been studied by (25a).

^vSpin splitting constants $\lambda_0 = +5.2787981 \text{ cm}^{-1}$, $\lambda_1 = +5.3105$, $\lambda_0 = -0.0056153 \text{ cm}^{-1}$, $\lambda_1 = -0.00572$ (39). For an improved representation of the rotational levels according to the intermediate case "c"-case "e" coupling model see (28)(33) (36); for an ab initio calculation of the spin-orbit part of λ (dominant contribution to the observed splitting) see (37). Rotational constants for $^{34}\text{S}^{16}\text{O}$, $^{32}\text{S}^{18}\text{O}$, $^{33}\text{S}^{16}\text{O}$ are

SO (continued):

given in (31)(32).

^wIn argon matrix.

^x $\mu_{el} = 1.55$ D from Stark effect of microwave sp. (6). The hf interaction due to ³³S has been studied by microwave (10) and ESR spectroscopy (13); see also (38).

- (1) Martin, PR 41, 167 (1932).
- (2) Norrish, Oldershaw, PRS A 242, 498 (1959).
- (2a) McGrath, McGarvey, JCP 37, 1574 (1962);
McGarvey, McGrath, PRS A 278, 490 (1964).
- (3) Abadie, Herman, CR 257, 2820 (1963).
- (4) Abadie, Herman, JQSRT 4, 195 (1964).
- (5) Colin, Goldfinger. Jeunehomme, TFS 60, 306 (1964).
- (6) Powell, Lide, JCP 41, 1413 (1964).
- (7) Winnewisser, Sastry, Cook, Gordy, JCP 41, 1687 (1964).
- (8) Carrington, Levy, Miller, PRS A 293, 108 (1966).
- (9) Daniels, Dorain, JCP 45, 26 (1966).
- (10) Amano, Hirota, Morino, JPSJ 22, 399 (1967).
- (11) Carrington, Levy, Miller, JCP 47, 3801 (1967).
- (12) Carrington, Levy, Miller, PRS A 298, 340 (1967).
- (13) Carrington, Levy, Miller, MP 13, 401 (1967).
- (14) Apparao, Narasimham, PIAS A 68, 173 (1968).
- (15) Colin, CJP 46, 1539 (1968).
- (16) Gaydon, DISSEN (1968).
- (17) Colin, CJP 47, 979 (1969).
- (18) Donovan, Husain, Jackson, TFS 65, 2930 (1969).
- (19) Smith, JQSRT 9, 1191 (1969).
- (20) Abadie, AP(Paris) 5, 227 (1970).
- (21) Saito, JCP 53, 2544 (1970).
- (22) Bouchoux, Marchand, Janin, SA A 27, 1909 (1971);
Bouchoux, Marchand, SA A 28, 1771 (1972).
- (23) Byfleet, Carrington, Russell, MP 20, 271 (1971).

SO (continued):

- (24) Donovan, Little, SpL 4, 213 (1971).
- (25) Jonathan, Smith, Ross, CPL 9, 217 (1971).
- (25a) Miller, JCP 54, 1658 (1971).
- (26) Smith, Liszt, JQSRT 11, 45 (1971).
- (26a) Uehara, MP 21, 407 (1971).
- (27) Smith, ApJ 176, 265 (1972).
- (27a) Brown, Uehara, MP 24, 1169 (1972).
- (28) Veseth, JP B 6, 1484 (1973).
- (29) Dyke, Golob, Jonathan, Morris, Okuda, Smith, JCS FT
II 70, 1818 (1974).
- (30) Hébert, Hodder, JP B 7, 2244 (1974).
- (31) Tiemann, JPCRD 3, 259 (1974).
- (32) Tiemann, JMS 51, 316 (1974).
- (33) Veseth, Lofthus, MP 27, 511 (1974).
- (34) Davies, Wayne, Stone, MP 28, 1409 (1974).
- (35) Hopkins, Brown, JCP 62, 2511 (1975).
- (36) Veseth, MP 29, 321 (1975).
- (37) Wayne, CPL 31, 97 (1975).
- (38) Veseth, JMS 52, 51 (1976).
- (39) Clark, De Lucia, JMS 60, 332 (1976).

$SO^+ : a_{D_0^0}(SO) + I.P.(S) - I.P.(SO).$

- (1) See ref. (29) of SO.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(88)Sr ⁷⁹ Br		$(\mu = 41.584947_1) \quad D_0^0 = 3.4_1 \text{ eV}^a$ V shaded emission bands in the region 17000 - 20000 cm^{-1} have been attributed to transitions from three additional states to A $^2\Pi$ and B $^2\Sigma$.							SEP 1977	
E $^2\Sigma^+$	32052.5	248.0	H 0.65					E \rightarrow X, V	32068.2 H	(4)
D $^2\Sigma^+$	28958.2	247.8	H 0.55					D \leftrightarrow X, V	28973.8 H	(3)(11)
C $^2\Pi$	24665.8 24343.7	205.2	H 0.49					C ^b \leftrightarrow X, R	24660.2 H 24338.1 H	(1)(3)(10) (11)
B $^2\Sigma^+$	15352.0	222.0	H 0.55					B ^b \leftrightarrow X, V	15354.7 H	(2)(3)
A $^2\Pi$	15000.7 14699.4	222.1	H 0.53					A ^b \leftrightarrow X, V	15003.5 H 14702.2 H	(2)(3)
X $^2\Sigma^+$	0	216.5	H 0.51							
(88)Sr ³⁵ Cl		$(\mu = 25.0170662) \quad D_0^0 = 4.1_6 \text{ eV}^a$							SEP 1977	
H $^2\Sigma^+$	34256.7	364.6	H 1.08					H \rightarrow B,	18562.7 H	(5)
								H \leftrightarrow X, V	34287.8 H	(4)(5)
G ($^2\Delta$)	34085.4 34059.6	356.7	H 1.0					G \rightarrow A,	18996.4 H 19264.8 H	(5)
F ($^2\Pi$)	32974.8 32905.9	354.2	H 1.09					F \rightarrow B,	17277.5 H 17208.4 H	(5)
								F \rightarrow A,	17884.6 H 18109.9 H	(5)
E $^2\Sigma^+$	32201.8	346.3	H 1.10					E \rightarrow A,	17396.1 H	(5)
								E \leftrightarrow X, V	32223.8 H	(4)(5)
D $^2\Sigma^+$	28822.9	344.8	H 1.04					D \rightarrow B,	13123.7 H	(5)
								D \rightarrow A,	13727.0 H 14021.8 H	(5)
								D \leftrightarrow X, V	28844.1 H	(4)(5)
C $^2\Pi$	25399.8 25244.6	283.4 282.1	H 0.92 H 0.89					C ^b \leftrightarrow X, R	25390.4 H 25234.5 H	(1)(2)(5)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(88)Sr ³⁵ Cl (continued)										
B $2\Sigma^+$	15719.5	306.4	H 0.98					$B^b \leftrightarrow X, v$	15721.5 ^c H 15713.1 ^c H	(1)(3)* (4) (7)
A 2Π	15112.6 14818.4	309.4	H 0.98					$A^b \leftrightarrow X, v$	15116.1 H 14821.9 H	(1)(2)(3)* (4)(5)(7)
X $2\Sigma^+$	0	302.3	H 0.95							

SrBr: ^aThermochemical value (mass-spectrom.) (12); in good agreement with the flame photometric value of (6)(7) but considerably below the lower limit to D_0^0 derived by (9) from the study of chemiluminescence spectra.

^bThe following radiative lifetimes have been measured by (8): A 34 ns, B 42 ns, C 29 ns.

- (1) Olmsted, ZWP 7, 300 (1906).
- (2) Hedfeld, ZP 68, 610 (1931).
- (3) Harrington, Dissertation (U. of California, 1942).
- (4) Reddy, Rao, IJPAP 4, 251 (1966).
- (5) Reddy, Reddy, Ashrafunnisa, Rao, CS 40, 317 (1971).
- (6) Gurvich, Ryabova, Khitrov, FSCS No. 8, 83 (1973).
- (7) Khitrov, Ryabova, Gurvich, HT(USSR) 11, 1005 (1973).
- (8) Dagdigian, Cruse, Zare, JCP 60, 2330 (1974).
- (9) Menzinger, CJC 52, 1688 (1974).
- (10) Joshi, Gopal, Pramāṇa 4, 276 (1975).
- (11) Puri, Mohan, CS 44, 152 (1975).
- (12) Hildenbrand, JCP 66, 3526 (1977).

SrCl: ^aThermochemical value (mass-spectrom.) (6), in very good agreement with the most recent flame photometric results of (8)(10). (9) place a lower limit to the dissociation energy at 4.2₉ eV based on their study of the Sr + Cl₂ chemiluminescent reaction.

^b(11) have measured the following radiative lifetimes: A 31 ns, B 39 ns, C 26 ns.

^cDouble heads on account of large spin doubling.

- (1) Parker, PR 47, 349 (1935).
- (2) More, Cornell, PR 53, 806 (1938).
- (3) Gatterer, RS 1, 153 (1942).
- (4) See ref. (3) of SrBr.
- (5) Novikov, Gurvich, OS(Engl. Transl.) 19, 76 (1965).
- (6) Hildenbrand, JCP 52, 5751 (1970).
- (7) Singh, Nair, Upadhyaya, Rai, OPA 3, 76 (1970).
- (8) Gurvich, Ryabova, Khitrov, Starovoitov, HT(USSR) 2, 261 (1971).
- (9) Jonah, Zare, CPL 2, 65 (1971).
- (10) See ref. (6) of SrBr.
- (11) See ref. (8) of SrBr.

State	T _e	ω _e		ω _e x _e	B _e	α _e	D _e (10 ⁻⁵ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
									Design.	ν ₀₀		
(88)Sr ¹⁹ F		(μ = 15.6221112) D ₀ ⁰ = 5.58 eV ^a									OCT 1977	
G (2Π)	34758.9	573.9	H	1.28	[0.26966] ^b	(0.00187)	[0.022 ₃]	[2.0004]	G←X, V	34795.4	H	(3)
F 2Σ ⁺	32823.7	598.5	H	3.42					F↔X, V	32871.96	Z	(3)(8)(9)
E 2Π	31615 31529.1	564.4	H	3.20					E↔X, V	31646.5 31560.4	H H	(3)(9)
D 2Σ ⁺	28296.6	552.1	H	2.15					D↔X, V	28322.0	H	(3)(9)
C 2Π	27445 27384.1	450.5 ^c	H	1.72 ^c	0.249396 ^{de}	0.001557	0.0252	2.08010	C↔X, R	27419.3 27358.8	H H	(1)(3)(9)
B 2Σ ⁺	17267.42	495.8 ^d	Z	2.3 ₄					B↔X, R	17264.10	Z	(1)(2)* (3) (4)(13)
A 2Π	15349.0 15068.3	507.3 ^c 507.9 ^c	H H	2.18 ^c 2.21 ^c					A ^f ↔X, V	15352.0 15071.6	H H	(1)(2)* (3) (9)
X 2Σ ⁺	0	502.4 ^{dg}	Z	2.2 ₇	0.250533 ^{dh}	0.001546	0.0249	2.07537	Rotation sp. ⁱ ESR sp. ^j			(14) (11)
(88)Sr ¹ H		(μ = 0.99640162) D ₀ ⁰ ≤ 1.66 eV ^a									SEP 1977	
Fragments of several additional absorption systems above 30000 cm ⁻¹ ; tentative rotational analyses.												(9)* (10) (16)* (17)*
F 2Σ ⁺	34096	[1337.0]	Z	(33) ^b	[4.0020] ^c	0.09 ₂	[13.84]	[2.0561]	F←X, V	34189.97	Z	(6)* (7)(9) (10)
C 2Σ ⁺	26230	1347	H	23.5	4.008 ^d	0.132	14	2.055	C↔X, V	26298.7	Z	(2)(4)(5) (8)*
D 2Σ ⁺	20847.6	1014.1	Z	15.4	1.925 ^e	0.024	3	2.965	D↔X, ^f R	20752.0	Z	(3)(5)
E 2Π					[3.869] [3.639] ^g		[20] [10]	[2.091] [2.156]	E→X, V	18960 18860	Z Z	(2)
B 2Σ ⁺	14340	[1193.0]	Z	(19) ^b	3.8788 ^h	0.0930	17.3	2.0885	B→X, V	14352.1	Z	(1)* (3)
A 2Π _r	i				[3.679] [3.668] ^j		[11.3] [13.3]	[2.144] [2.148]	A→X, V	13653 13360	Z Z	(1)*
X 2Σ ⁺	0	1206.2	Z	17.0	3.6751 ^k	0.0814	[13.5] ^l	2.1456	ESR sp. ^m			(12)

SrF: ^aThermochemical value (mass-spectrom.)(10). Re-evaluation by (10) of the earlier data of (5)(6) gives $D_0^0 = 5.45$ eV; flame photometric value 5.7_2 eV (7).
^bSpin doubling constant $|\gamma| = 0.043$ (8).
^cVibrational constants of (9).
^dConstants for $^{88}\text{Sr}^{19}\text{F}$ (13)(14).
^eLarge spin doubling, $\gamma = -0.1353_4$ cm^{-1} (14).
^fRadiative lifetime $\tau = 23$ ns (12).
^gSimilar constants are obtained from bandhead measurements in D-X, E-X, F-X: $w_e'' = 501.3$, $w_e''x_e'' = 2.2_5$ (averaged values).
^hSpin-rotation interaction $\gamma = +0.00249$ (14).
ⁱMicrowave optical double resonance.
^jIn Ne and Ar matrices at 4 K.

(1) Johnson, PRS A 122, 161 (1929).
 (2) Harvey, PRS A 133, 336 (1931).
 (3) Fowler, PR 59, 645 (1941).
 (4) Ahrens, PR 74, 74 (1948).
 (5) Blue, Green, Ehlert, Margrave, Nature 199, 804 (1963).
 (6) Ehlert, Blue, Green, Margrave, JCP 41, 2250 (1964).
 (7) Ryabova, Gurvich, HT(USSR) 2, 749 (1964).
 (8) Barrow, Beale, CC (1967), 606.
 (9) Novikov, Gurvich, OS(Engl. Transl.) 22, 395 (1967).
 (10) Hildenbrand, JCP 48, 3657 (1968).
 (11) Knight, Easley, Weltner, Wilson, JCP 54, 322 (1971).
 (12) Dagdigian, Cruse, Zare, JCP 60, 2330 (1974).
 (13) Steimle, Domaille, Harris, JMS 68, 134 (1977).
 (14) Domaille, Steimle, Harris, JMS 68, 146 (1977).

Sr¹H, Sr²H:

^aFrom the predissociation in $\text{C } ^2\Sigma^+$ assuming dissociation into $^3\text{P}_0 + ^2\text{S}$.
^bFrom isotope relations.
^cSpin doubling constant $\gamma_0 = +0.076$. All lines are diffuse owing to predissociation.
^dBreaking-off in emission at low pressure above $N'=19$ and 4 in $v'=0$ and 1, respectively (8). Perturbations.
^eStrong perturbations.
^fFranck-Condon factors (11).
^gPerturbations.
^hSpin doubling constant $\gamma_0 = -3.81$ [for $N < 10$ (3)]. For a more elaborate evaluation of the spin splitting including higher-order correction terms see (14).
ⁱ $A_0 \approx +300$. See also ^j.
^jVery large Λ -type doubling, see (1)(15). The constants given here are effective values; see, however, (13) who has evaluated the true constants by taking into account several usually neglected corrections to the rotational energy formulae for a $^2\Pi$ state.
^kFrom (3); spin doubling constant $\gamma_0 = +0.122$. (6) give $B_0 = 3.6336$, $D_0 = 13.39 \times 10^{-5}$.
^l $D_1 = 12.9 \times 10^{-5}$.
^mIn argon matrix at 4 K.

(continued p. 628)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(88)Sr²H		$(\mu = 1.96898856) \quad D_0^0 \leq 1.70 \text{ eV}^a$ Fragments of additional absorption systems above 30000 cm^{-1} ; tentative rotational analyses.								SEP 1977
F $2\Sigma^+$	34097	[964.6]	Z (17) ^b	[2.0334] ⁿ	0.032	[3.47]	[2.0519]	F \leftarrow X, V	34164.87 Z	(9)(10)(16)* (17)*
C $2\Sigma^+$	26226	[943]	Z (11.9) ^o	1.98 ^p	0.03	[2.5]	2.08	C \rightarrow X, V	26279 Z	(6)(7)(9) (10)
B $2\Sigma^+$	14335	[857]	Z (10) ^b	1.9426 ^q	0.0349	[4.02] ^r	2.0994	B \rightarrow X, V	14343.9 Z	(3)(8)* (3)
X $2\Sigma^+$	0	[841]	Z (8.6) ^o	1.8609 ^s	0.0292	[3.47] ^t	2.1449			
(89)Sr¹²⁷I		$(\mu = 51.932462_5) \quad D_0^0 \geq 2.8_2 \text{ eV}^a$								SEP 1977
F		210.4	H 0.40					F \rightarrow A or B, V	19902.1 H 19599.3 H	(12)
D (2Σ)	28944.0	200.4	H 0.50					D \rightarrow X, V	28957.1 H	(8)* (10)
C (2Π)	23223.4 22666.1	168.5 170.9	H 0.40 H 0.36					C ^b \leftrightarrow X, R	23220.6 H 22664.5 H	(1)(2)(5)*
B (2Σ) ^c	14815.9	182.2	H 0.37					B ^b \rightarrow X, V	14820.1 H	(9)*
A (2Π) ^c	14748.8 14422.7	179.5 182.3	H 0.32 H 0.54					A ^b \leftrightarrow X, V	14751.7 H 14427.0 H	(1)(4)(6) (9)*
X $2\Sigma^+$	0	174.1 ^d	H 0.35 ^d							

Sr¹H, Sr²H (continued):ⁿSpin doubling constant $\gamma_0 = +0.035_7$.^oFrom the value for Sr¹H.^pBreaking-off above N'=29 and 19 in $v'=0$ and 1, respectively (8). Strong perturbations.^qSpin doubling constant $\gamma_0 = -2.01$ [for N<10 (3)]. See ^h.^r $D_1 = 3.81 \times 10^{-5}$.Sr¹H, Sr²H (continued):^sSpin doubling constant $\gamma_0 = +0.061_3$.^t $D_1 = 3.64 \times 10^{-5}$.(1) Watson, Fredrickson, PR 32, 765 (1932).(2) Fredrickson, Hogan, Watson, PR 48, 602 (1935).(3) Watson, Fredrickson, Hogan, PR 49, 150 (1936).(4) Humphreys, Fredrickson, PR 50, 542 (1936).

Sr¹H, Sr²H (continued):

- (5) More, Cornell, PR 53, 806 (1938).
- (6) Edvinsson, Kopp, Lindgren, Åslund, AF 25, 95 (1963).
- (7) Khan, PPS 81, 1047 (1963).
- (8) Khan, PPS 82, 564 (1963).
- (9) Khan, PPS 89, 165 (1966).
- (10) Khan, Butt, JP B 1, 745 (1968).
- (11) Singh, Srivastava, JQSRT 8, 1443 (1968).
- (12) Knight, Weltner, JCP 54, 3875 (1971).
- (13) Veseth, JMS 38, 228 (1971).
- (14) Veseth, MP 20, 1057 (1971).
- (15) Veseth, MP 21, 287 (1971).
- (16) Khan, Rafi, Hussainee, JP B 2, 1953 (1976).
- (17) Khan, Rafi, Khan, Baig, JP B 2, 2313 (1976); 10, 111 (1977).

SrI: ^aFrom a reactive scattering study of the Sr+HI reaction by the crossed molecular beam technique (7). The ionic model calculations of (3) predict $D_0^0 \approx 2.92$ eV.

^bRadiative lifetimes measured by (11): A 42 ns, B 46 ns,

SrI (continued):

C 36 ns. There seems to be some uncertainty concerning the correct identification of the B state emission.

^cAccording to (9) the tentative assignments for these two states or substates (i.e. Σ and Π) should be reversed.

^dAverage values for the lower state constants of A...D→X.

- (1) Walters, Barratt, PRS A 118, 120 (1928).
- (2) Mesnage, AP(Paris) 12, 5 (1939).
- (3) Krasnov, Karaseva, OS(Engl. Transl.) 19, 14 (1965).
- (4) Shukla, IJPAP 8, 855 (1970).
- (5) Reddy, Reddy, Rao, JP B 4, 574 (1971).
- (6) Reddy, Reddy, Rao, Rao, CS 40, 186 (1971).
- (7) Mims, Lin, Herm, JCP 57, 3099 (1972).
- (8) Shah, Patel, Darji, JP B 6, 1344 (1973).
- (9) Ashrafunnisa, Rao, Rao, JP B 6, 1503 (1973).
- (10) Ashrafunnisa, Rao, Rao, JP B 6, 2653 (1973).
- (11) Dagdigian, Cruse, Zare, JCP 60, 2330 (1974).
- (12) Kamalasanan, IJPAP 13, 124 (1975).

SrS (continued from p. 631):

- (1) Marquart, Berkowitz, JCP 39, 283 (1963).
- (2) Colin, Goldfinger, Jeunehomme, TFS 60, 306 (1964).
- (3) Cater, Johnson, JCP 47, 5353 (1967).
- (4) Marciano, Barrow, TFS 66, 1917 (1970).

SrSe (Table on p. 630):

^aThermochemical value (mass-spectrom.)(1), corrected for new value of $D_0^0(\text{Se}_2)$.

- (1) Berkowitz, Chupka, JCP 45, 4289 (1966).

State	T_e	w_e		$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References	
									Design.	ν_{00}		
$^{88}\text{Sr}^{16}\text{O}$												
		$\mu = 13.5325861_5$		$D_0^0 = 4.8_8 \text{ eV}^a$								SEP 1977 A
C $^1\Sigma^+$	28632.7	480.2	Z	2.6	0.2742^b	0.0021	3.5	2.131	$C \rightarrow X, ^c$	R 28546.4 ₃ Z	(1)(9)*	
B $^1\Pi$	24701.0	519.9 ₁	Z	3.2 ₄	0.2937	0.0015	5.0	2.059	$B \rightarrow X, ^c$	R 24634.4 Z	(1)(7)* (8)	
Unclassified bands in the regions 14700-15700 and 16600-16900 cm^{-1} . The emitter of these bands has long been in doubt (13)(32); in flames, and in arcs in water vapour, strong bands attributed to SrOH occur in the same regions (11)(14). The bands have recently been observed in dry $\text{Sr} + \text{N}_2\text{O} + \text{CO}$ (or N_2^*) flames, both in emission and in absorption (33)(34)(35), and have tentatively been attributed to the transitions $^3\Delta \leftrightarrow a^3\Pi$ and $^1\Delta, ^1\Sigma^- \leftrightarrow A^1\Pi$ of SrO.												
A $^1\Sigma^+$	10886.59	619.5 ₈	Z	0.8_9^d	0.3047_1^e	0.0011_2	3.2	2.021_9	$A \rightarrow X, ^f$	R 10870.40 Z	(2)* (4)* (5) (12)* (16)* (21)	
A' $^1\Pi$	9400	472.8_8^g	H	2.06	0.256_5^h	0.0017		2.20_4	$A' \rightarrow X, R$	9310 H	(29)(31)	
a $^3\Pi_1$	9149^i	463.5		1.61	0.2584	0.0020		2.196				
X $^1\Sigma^+$	0	653.4_9	Z	3.96	0.33798_0	0.00219_4	3.6	1.91983	IR spectrum ^j Microwave and rf sp. ^{kl}		(28) (19)	
$^{88}\text{Sr}^{32}\text{S}$												
		$\mu = 23.4449370$		$D_0^0 = 3.48 \text{ eV}^a$								SEP 1977
B $^1\Sigma^+$	39332.1	286.8_0	Z	0.84	0.10566^b	0.00032_0	0.575	2.608_7	$B \leftarrow X, R$	39281.4_2 Z	(4)*	
X $^1\Sigma^+$	0	388.38	Z	1.31	0.12072	0.00044_0	0.475	2.4405				
$(^{88}\text{Sr}^{80}\text{Se})$												
		$(\mu = 41.860458_9)$		$D_0^0 \approx 2.9 \text{ eV}^a$								SEP 1977

SrO: ^aFrom the appearance threshold of SrO in a crossed-beam study of the $\text{Sr} + \text{O}_2$ reaction (25); the interpretation of the chemiluminescence spectrum resulting from the reaction $\text{Sr} + \text{ClO}_2$ in a similar experiment (30) leads to $D_0^0 \geq 4.6_7 \text{ eV}$. Good agreement with the flame-photometric results ($D_0^0 = 4.8_1 \text{ eV}$) of (15) and (10), the latter re-

calculated for a $^1\Sigma$ state, and with the thermochemical value ($D_0^0 = 4.9_0 \text{ eV}$) of (6). Flame-photometric values of (20)(26) are lower, even when recalculated with a $^1\Sigma$ ground state, and are close to the mass-spectrometric value of (18) ($D_0^0 = 4.4_3 \text{ eV}$). Earlier references have been reviewed in these papers; see also (22).

SrO (continued):

^bSeveral perturbations (9).

^cRKR Franck-Condon factors (24).

^d $w_{e'v_e} = -0.054$. Bandheads in the region 8959 - 9166 cm^{-1} , originally (12) attributed to a new system of SrO, have been shown (21) to belong to the A \rightarrow X 0-3 sequence.

^eNumerous perturbations by levels of a $^3\Pi_i$ and A' $^1\Pi$ (5)
^fFranck-Condon factors (17). | (27).

^gVibrational numbering (29) confirmed by isotope studies (31).

^hThe rotational constants have been derived (29) with the help of information gained from the analysis of perturbations in A $^1\Sigma^+$ (5)(27).

ⁱA = -70; all constants for this state derived by (27) from perturbations in A $^1\Sigma^+$ (5).

^jIn nitrogen matrices.

^kBy the molecular beam electric resonance method. $\mu_{el} = 8.913 - 0.026(v + \frac{1}{2})$ D (19).

^lAb initio calculations of various ground state properties (23).

(1) Mahanti, PR 42, 609 (1932).

(2) Mahla, ZP 81, 625 (1933).

(3) Gatterer, RS 1, 153 (1942).

(4) Almkvist, Lagerqvist, AF 1, 477 (1949).

(5) Almkvist, Lagerqvist, AF 2, 233 (1950).

(6) Drummond, Barrow, TFS 47, 1275 (1951).

(7) Kovács, Budó, APH 1, 469 (1952); AP(Leipzig) 12, 17 (1953).

(8) Deézsi, Koczka, Mátrai, APH 3, 95 (1953).

(9) Lagerqvist, Almkvist, AF 8, 481 (1954).

(10) Lagerqvist, Huldt, ZN 2 a, 991 (1954).

(11) Lagerqvist, Huldt, Naturw. 42, 365 (1955).

SrO (continued):

(12) Lagerqvist, Selin, AF 11, 323 (1956).

(13) Charton, Gaydon, PPS A 69, 520 (1956).

(14) Huldt, Lagerqvist, AF 11, 347 (1956).

(15) Veits, Gurvich, OS 1, 22 (1956); 2, 145 (1957); ZFK 31, 2306 (1957).

(16) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(17) Nicholls, JRNBS A 66, 227 (1962).

(18) Drowart, Exsteen, Verhaegen, TFS 60, 1920 (1964).

(19) Kaufman, Wharton, Klemperer, JCP 43, 943 (1965).

(20) Kalff, Hollander, Alkemade, JCP 43, 2299 (1965).

(21) Brewer, Hauge, JMS 25, 330 (1968).

(22) Gaydon, DISSEN (1968), p. 242.

(23) Yoshimine, JPSJ 25, 1100 (1968).

(24) Liszt, Smith, JQSRT 11, 1043 (1971).

(25) Batalli-Cosmovici, Michel, CPL 16, 77 (1972).

(26) Kalff, Alkemade, JCP 59, 2572 (1973).

(27) Field, JCP 60, 2400 (1974).

(28) Ault, Andrews, JCP 62, 2320 (1975).

(29) Capelle, Broida, Field, JCP 62, 3131 (1975).

(30) Engelke, Sander, Zare, JCP 65, 1146 (1976).

(31) Hecht, JCP 65, 5026 (1976).

(32) Pearse, Gaydon, IDSPEC (1976), p. 339.

(33) Benard, Slafer, Hecht, JCP 66, 1012 (1977).

(34) Eckstrom, Barker, Hawley, Reilly, AO 16, 2102 (1977).

(35) Benard, Slafer, Love, Lee, AO 16, 2108 (1977).

SrS: ^aThermochemical value (mass-spectrom.)(1)(2)(3).

^bExtensive perturbations.

References on p.629 .

SrSe: See p.629 .

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{181}\text{Ta}^{16}\text{O}$										
$\mu = 14.6958722_5$ $D_0^0 = 8.2 \text{ eV}^a$										
Weak emission bands at 35476 and 36379 cm^{-1} , no analysis.										
V ($^2\Delta$) 5/2						$[0.375]^{bc}$	$[3.3]$	$[1.74_9]$	$V \rightarrow X_2$, R 33280 ^b	(2) (7)
U ($^2\Delta$) 5/2						$[0.3715]^c$	$[3.3]$	$[1.757_2]$	$U \rightarrow X_2$, R 33110	(2) (7)
T ($^2\Delta$) 5/2 35954		(891)				$[0.37688]^d$	$[2.70]$	$[1.7446_1]$	$T \rightarrow X_2$, R 32380.7 ₇	Z (7)
S ($^2\Delta$) 5/2 35864		(871)				$[0.37536]^d$	$[2.79]$	$[1.7481_4]$	$S \rightarrow X_2$, R 32280.4 ₀	Z (7)
R ($^2\Delta$) 3/2 32445		(885)				$[0.38393]^d$	$[2.89]^e$	$[1.7285_2]$	$R \rightarrow X_1$, R 32373.6 ₀	Z (7)
Q (29306)		$[(895)]^f$							$Q \leftarrow X_1$, (29240) ^f	(6)
Q' ($^2\Delta$) 5/2 27353.0		$[896.1]$	Z (4.07)		0.38183 ₄ ^g	0.00219	$[2.744]$	1.73326	$Q' \rightarrow X_2$, R 23785.2 ₀	Z (7)
P ($^2\Delta$) 3/2 26736.19		902.68	Z 4.08		0.37750 ₀ ^h	0.00181	$[2.573]$	1.74318	$P \leftrightarrow X_1$, R 26673.0 ₄	Z (1)(2)* (4) (6)(7)
O (26342)		(913) ^f	(4.5)						$O \leftarrow X_1$, (26284) ^f	(6)
O' ($^2\phi$) 7/2 26186		(899)			$[0.381304]$		$[2.745]$	$[1.73446_2]$	$O' \rightarrow X_2$, R 22616.0 ₇	Z (7)
N ($^2\Pi$) 3/2 25657		(900)			$[0.37720_7]$		$[2.64_9]$	$[1.74386]$	$N \rightarrow X_2$, R 22087.7 ₀	Z (7)
									$N \leftrightarrow X_1$, R 25593.1 ₃	Z (6)(7)
M ($^2\phi$) 5/2 24123.7		$[890.31]$	Z 4.1 H		0.37706 ₄	0.00184	$[2.635]$	1.74419	$M \leftrightarrow X_1$, R 24058.4 ₂	Z (2)* (4)(6) (7)
L ($^2\Pi$) 1/2 23408.3		$[887.70]$	Z 4.1 H		0.37742 ₄ ⁱ	0.00195	$[2.70_6]$	1.74335	$L \leftrightarrow X_1$, R 23341.7 ₄	Z (2)* (4)(6) (7)
K' ($^2\phi$) 7/2 22981.5 ₈		903.06	Z 3.56		0.38081	0.00192	$[2.756]$	1.7355 ₉	$K' \rightarrow X_2$, R 19413.3 ₂	Z (7)
K (22396)		(901.7) ^f	(3.3 ₄)						$K \leftrightarrow X_1$, (22333) ^f	(6)
J (22196)		(892) ^f	(3)						$J \leftarrow X_1$, (22128) ^f	(6)
(I) Ne matrix emission and absorption spectra suggest the existence of an additional state close to H.										(6)
H (20868)		$[(900)]^j$							$H \leftrightarrow X_1$, (20805) ^j	(6)
G									$G \leftarrow X_1$, (18007) ^f	(6)
F (16770)		$[(922)]^f$							$F \leftarrow X_1$, (16718) ^f	(6)
		Incompletely analysed emission band.							R 16051	Z (7)
E ($^2\phi$) 5/2 15928		(935) ^f	(5)		$[0.38618]^k$		$[3.2_6]$	$[1.7234_8]$	$E \leftrightarrow X_1$ R 15880.6 ₂	Z (6)(7)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{181}\text{Ta}^{16}\text{O}$ (continued)										
D	(14437)	(943) ^l						D \leftrightarrow X ₁ , (14395) ^{fm}	(6)(7)	
C (² Δ) 3/2	13612	(942)		[0.38754 ₇]		[2.62 ₄]	[1.72044]	C \leftrightarrow X ₁ , R 13569.27 Z	(6)(7)	
B (² ϕ) 5/2	12900	(931)		[0.38685 ₁]		[2.67 ₄]	[1.72198]	B \leftrightarrow X ₁ , R 12852.02 Z	(6)(7)	
A	(12134)	[(939)] ⁿ						A \leftrightarrow X ₁ , (12090) ^o	(6)(7)	
A* (² Π) 1/2				[0.389]			[1.71 ₇]	A* \rightarrow X ₁ , R 11062 (Z)	(7)	
A'' (² Δ) 3/2	10908	(933)		[0.38729 ₁]		[2.66 ₈]	[1.72100]	A'' \rightarrow X ₁ , R 10860.95 Z	(7)	
X ₂ (² Δ) 5/2	3504.39	1030.81	Z 3.59	0.40358 ₄	0.00187	[2.503]	1.68591			
X ₁ 3/2	0	1028.69	Z 3.51	0.40284 ₀	0.00182	[2.450]	1.68746	IR spectrum ^p	(6)	
$^{181}\text{Ta}^{16}\text{O}^+?$										JUN 1975
A	17933	(952)		0.3906	0.0022	2.63	1.713 ₇	A \rightarrow X, ^a R 17880.41 Z	(1)	
(X)	0	[1051.12]	Z (3.41)	0.4128 ₇	0.0018 ₁	2.52	1.6668			

TaO: ^aAverage of two thermochemical values (mass-spectrom.)
^bThis level could possibly be T(v=1). (3)(5).
^cExtensive perturbations.
^dPerturbations.
^e(7) give 2.289 which appears to be a misprint.
^fFrom the Ne matrix absorption spectrum.
^gPerturbations in v=0.
^hv=1 perturbed by a state of higher B value.
ⁱ Λ -type doubling $\Delta v(v=0) = 0.0927(J+\frac{1}{2})$.
^jFrom Ne matrix absorption and emission spectra.
^kPerturbed by a state of larger B value.
^lCalculated from Ta¹⁸O frequency in neon.
^mIn the gas phase probably at 14362 cm⁻¹.
ⁿFrom the Ar matrix absorption spectrum.

TaO (continued):
^oFrom (7); the observed band is too weak for analysis.
^pIn rare gas matrices.
(1) Premaswarup, IJP 29, 109 (1955).
(2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
(3) Inghram, Chupka, Berkowitz, JCP 27, 569 (1957).
(4) Premaswarup, Barrow, Nature 180, 602 (1957).
(5) Krikorian, Carpenter, JPC 69, 4399 (1965).
(6) Weltner, McLeod, JCP 42, 882 (1965).
(7) Cheetham, Barrow, TFS 63, 1835 (1967).
TaO⁺: ^aP, Q, R branches, probably singlet system.
(1) See ref. (7) of TaO.

Tb₂: ^aThermochemical value (mass-spectrom.)(1).
(1) Kordis, Gingerich, Seyse, JCP 61, 5114 (1974).

TbO: ^aThermochemical value (mass-spectrom.)(3), re-calculated (4).

^bFrom the IR sp. of Tb¹⁶O in argon at 15 K; for Tb¹⁸O at 781.7. Derived constants $\omega_e = 828.4$, $\omega_e x_e = 2.1$ (5).

(1) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(2) Herrmann, Alkemade, "Chemical Analysis by Flame Photometry", 2nd rev. ed., Interscience (1963).

(3) Ames, Walsh, White, JPC 71, 2707 (1967).

(4) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

(5) Gabelnick, Reedy, Chasanov, JCP 60, 1167 (1974).

Te₂, Te₂⁺:

^aWeighted mean (17) of several values obtained by spectroscopic (14)(17) and thermochemical (12)(18) methods and from a photoionization threshold (13).

^bBy photoionization mass-spectrometry (13)(16). Similar values from the photoelectron spectrum (20)(23).

^cConstants for the only observed vibrational level of this state, from laser-excited fluorescence spectra. The v numbering is unknown (probably $6 \leq v' \leq 10$).

^dThe vibrational numbering adopted here was first suggested by (4) and has recently been confirmed by isotope studies (14)(15)(17); v' has been increased by +3 units compared to the numbering used by (1)(9a)(10).

^e $\omega_e y_e = -0.01109$ (for $v < 20$, see ^f).

^fNumerous local perturbations. A much stronger homogeneous perturbation affects levels with $v \geq 20$ (14)(15)(17). Predissociation above $v=23$ (2)(4), i.e. at $\sim 25600 \text{ cm}^{-1}$ above $X_1 O_g^+(v=0)$; induced predissociation below this limit (3)(4)(6); accidental prediss. of the vibrational type (9).

^gRot. analyses of bands of ¹²⁸Te₂ (17), extended by (19).

Te₂, Te₂⁺ (continued):

^hContinuous emission with maximum at 19200 cm^{-1} has been interpreted as recombination continuum (5).

ⁱ $\omega_e y_e = -0.003892$.

^jPotential curves (21).

^k $r_e = +2.2 \times 10^{-7}$.

^l $\omega_e y_e = -0.00055$ (17).

^mFrom $D_0^0(\text{Te}_2) + \text{I.P.}(\text{Te}) - \text{I.P.}(\text{Te}_2)$.

(1) Rosen, ZP 43, 69 (1927).

(2) Hirschlaff, ZP 75, 315 (1932).

(3) Kondratjew, Lauris, ZP 92, 741 (1934).

(4) Olsson, ZP 95, 215 (1935); Dissertation (Stockholm,

(5) Rompe, ZP 101, 214 (1936); PZ 37, 807 (1936). 1938).

(6) Olsson, CR 204, 1182 (1937).

(7) Choong, AP(Paris) (11) 10, 173 (1938).

(8) Migeotte, MSRL (4) 5, 3 (1942).

(9) Rosen, PR 68, 124 (1945).

(9a) Herzberg, MOLSPEC 1 (1950).

(10) Prasad, Rao, IJP 28, 549 (1954).

(11) du Parc, Barrow, CC (1966), p. 270.

(12) Budininkas, Edwards, Wahlbeck, JCP 48, 2870 (1968); 51,

(13) Berkowitz, Chupka, JCP 50, 4245 (1969). 1686 (1969)

(14) Jha, Rao, CPL 3, 175 (1969). (erratum).

(15) Jha, Subbaram, Rao, JMS 32, 383 (1969).

(16) Guyon, Berkowitz, JCP 54, 1814 (1971).

(17) Barrow, du Parc, PRS A 327, 279 (1972).

(18) Smoes, Mandy, Auwera-Mahieu, Drowart, BSCB 81, 45 (1972).

(19) Yee, Barrow, JCS FT II 68, 1397 (1972).

(20) Berkowitz, JCP 62, 4074 (1975).

(21) Rao, Rao, Rao, SpL 8, 745 (1975).

(22) Stone, Barrow, CJP 53, 1976 (1975).

(23) Streets, Berkowitz, JESRP 2, 269 (1976).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
($^{130}\text{Te}^{79}\text{Br}$)											
		$(\mu = 49.093760_6)$								NOV 1977	
B	(43125) ^a	314.2	H	0.5				B \leftarrow X,	V 41430	H	(1)*
X ($^2\Pi_i$)	(1718) ^a ₀	267.4	H	0.7					43148	H	
($^{130}\text{Te}^{35}\text{Cl}$)											
		$(\mu = 27.5522041)$								NOV 1977	
B	(44262) ^a	458	H	1.5				B \leftarrow X,	V 42624	H	(1)*
X ($^2\Pi_i$)	(1674) ^a ₀	[386]	H						44298	H	
($^{130}\text{Te}^1\text{H}$)											
		$(\mu = 1.00006661)$								NOV 1977	
		I.P. = 9.0_9 eV^a									
T	#	Very strong.	}	Only single absorption bands have been observed without vibrational structure. According to (2) none of the bands shows any significant shift on deuteration.				T \leftarrow X ₁ ,	69589	}	(2)*
S								S \leftarrow X ₁ ,	68729		
R								R \leftarrow X ₁ ,	67797		
Q								Q \leftarrow X ₁ ,	66711		
P								P \leftarrow X ₁ ,	62150		
O								O \leftarrow X ₁ ,	60753		
N								N \leftarrow X ₂ ,	56850		
H								N \leftarrow X ₁ ,	60680		
D								H \leftarrow X ₁ ,	58824		
C								D \leftarrow X ₁ ,	55006		
B								C \leftarrow X ₂ ,	45872		
X ₂ ($^2\Pi_1$)	(3830) ^b	Very strong.	}					C \leftarrow X ₁ ,	49702	(1)	
X ₁	₀							B \leftarrow X ₁ ,	46404		
		[5.56]								EPR sp.	
								[1.74 ₁]			

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(130)Te¹²⁷I		$(\mu = 64.193905_3)$								NOV 1977
C	43658	251.8	H 0.5					C← X, V 43675	H	(1)*
B	41057	260.2	H 1.4					B← X, V (39263) ^a 41078	H	(1)*
X (² Π_1)	(1815) ^a 0	217.3	H 0.6							

TeBr, TeCl:

^aAssuming that there is no spin-orbit splitting in the B state.

(1) Oldershaw, Robinson, JMS 37, 314 (1971).

Te¹H: ^aFrom a tentative interpretation of several Rydberg series (e.g. C,P,Q,...) by (2).

^bFrom the interpretation of the VUV absorption spectrum (2); from the paramagnetic resonance spectrum (1) obtains $A_0 = -2250$.

(1) Radford, JCP 40, 2732 (1964).

(2) Donovan, Little, Konstantatos, JCS FT II 68, 1812 (1972).

TeI: ^aTentative, based on a single band head.

(1) Oldershaw, Robinson, TFS 67, 907 (1971).

TeSe (see p.639):

^aThermochemical value (mass-spectrom.)(1), corrected for new values of $D_0^0(\text{Se}_2)$ and $D_0^0(\text{Te}_2)$.

^bThe band structure is somewhat diffuse suggesting predissociation (2)(3).

^cAll constants for these states are derived from laser-excited fluorescence spectra. In carrying out the analysis it was necessary to assume the value of the rotational constant B_e for the ground state (3), see ^f.

^dFrom the $B_1 \rightarrow X_1$ and $B_1 \rightarrow X_2$ fluorescence series.

^eCombined results from fluorescence and absorption spectra.

^fEstimated value (3) assuming $r_e(\text{TeSe}) \approx \frac{1}{2}[r_e(\text{Te}_2) + r_e(\text{Se}_2)]$.

(1) Porter, Spencer, JCP 32, 943 (1960).

(2) Joshi, Sharma, PPS 20, 1159 (1967).

(3) Ahmed, Barrow, Yee, JP B 8, 649 (1975).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	ν_{00}		
$^{130}\text{Te}^{16}\text{O}$		$\mu = 14.2414174_5$ $D_0^0 \leq 3.90 \text{ eV}^a$ I.P. = 8.72 eV^b								NOV 1977	
		Fragment of an absorption system in the region $32700 - 36000 \text{ cm}^{-1}$; it is not certain that these bands are due to TeO .								(1)	
A_2 1	[28719]	^c		[0.2771] ^d	(0.004)	[2]	[2.067]	$A_2 \rightarrow X_2$, R	27641.9_5 Z	(2)* (3)*	
A_1 0 ⁺	(28212)	[444.95] Z	e	0.2760 ^{df}	0.0052	4	2.071	$A_1 \leftrightarrow X_1$, R	28037.0_4 Z	(2)* (3)*	
		Unclassified emission bands $16000 - 20000 \text{ cm}^{-1}$.								(2)	
X_2 1	679 ^g	798.06	Z	4.00	0.3564 ^h	0.00236	3	1.822 ₄			
X_1 0 ⁺	0	797.11	Z	4.00	0.3554	0.00237	2.7	1.825 ₀			
$(^{130})\text{Te}^{16}\text{O}^+$		$D_0^0 \leq 4.19 \text{ eV}^i$								NOV 1977	
$\left. \begin{array}{l} ({}^2\Pi) \\ B ({}^2\Sigma) \\ b ({}^4\Sigma) \\ A ({}^2\Pi) \\ a ({}^4\Pi) \\ X ({}^2\Pi) \end{array} \right\}$	$\left. \begin{array}{l} (38470) \\ 26450 \\ (19760) \\ 16780 \\ (4840) \\ 0 \end{array} \right\}$	From the photoelectron spectrum (5). Identifications are tentative, no vibrational structure was observed. Numbers in parentheses refer to peaks overlapped by impurities.									
$^{130}\text{Te}^{32}\text{S}$		$\mu = 25.6573697$ $D_0^0 = (3.5) \text{ eV}^a$								NOV 1977	
D_2	x + 42199	[526]	H					$D_2 \leftarrow X_2$, ^b V	42226 H	(1)*	
D_1	43283	524.2	H	0.8				$D_1 \leftarrow X_1$, V	43310 H	(1)*	
C 0 ⁺				[0.08115] ^c		[3.5] ^c	[2.845 ₄] ^c	$C \leftarrow X_1$, R	26886.96 ^c Z	(3)	
B 0 ⁺	24530	250.3 ^d	Z	(3.37)	0.1027 ^d	0.00120	(1.1)	2.529	$B \leftarrow X_1$, R	24419 ^d Z	(3)
A 0 ⁺	23549	204.2 ^d	Z	1.018	0.0976 ₂ ^d	0.00075	(0.7)	2.594	$A \leftarrow X_1$, R	23415.4 ^d Z	(3)
X_2 1	x ^e	(472)	H								
X_1 0 ⁺	0	471.18 ^f	Z	(1.57)	0.13216 ^g	0.00050 ^g	0.40	2.2297			

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References	
								Design.	v ₀₀		
¹²⁸ Te ⁷⁸ Se		μ = 48.420396 ₁ D ₀ ⁰ = 3.0 eV ^a Unclassified absorption bands 43900 - 46500 cm ⁻¹ .							NOV 1977		
D ₂	42232.3	353.3	H 1.0	Double-headed bands ^b				D ₂ ←X ₂ , v	40703.0	H ^Q	(2)
D ₁	42168.4	355.6	H 1.0					D ₁ ←X ₁ , v	42188.0	H ^Q	(2)* (3)
C 1	c			B ₂ = 0.0477			r ₂ = 2.70 ₂	C→X ₂ , v(2-0) =	22490		(3)
B ₂ 1	23596	[191.5]		[0.048]			[2.69]	B ₂ →X ₂ ,	21986		(3)
B ₁ 0 ⁺	23393	[189]		0.0497			2.64 ₇	B ₁ →X ₂ ,	21781		(3)
								B ₁ →X ₁ ,	23329.1		(3)
A 0 ⁺	c							A→X ₁ , v(2-0) =	22052		(3)
X ₂ 1	1547.2 ^d	317.39 ^e	0.7175	(0.0619) ^f			(2.37 ₂)				
X ₁ 0 ⁺	0	316.24 ^e	0.738	(0.0619) ^f	(0.00018)	(0.095)	(2.37 ₂)				

TeO, TeO⁺:

^aFrom the predissociation in $A_1 0^+$ (see ^f).

^bFrom the photoelectron spectrum (5).

^c(3) give, without details, $\Delta G(\frac{1}{2}) \approx 458$ for ^{128}TeO . (2), by contrast, suggest $w_e = 408$, $w_e x_e = 4.0$. According to (3) this state is predissociated between $v=2$ and 3.

^dExtensive perturbations.

^e $\Delta G(3/2) = 409.9$, $\Delta G(5/2) = 393.4$, $\Delta G(7/2) = 364.53$. From $v=3$ to 10 the vibrational intervals are quite well represented by $w_e = 410.71$, $w_e x_e = 5.772$; large deviations occur below and above these limits. Vibrational levels observed to $v=15$. The v' numbering has been established from isotope shifts (3) and has been increased by +3 units compared to the numbering used by (1) and (2).

^fAbsorption lines become diffuse above $J' \approx 42$ and 14 in $v'=9$ and 10, respectively; the highest observed level in emission is $v'=9$. The predissociation limit ($\sim 31450 \text{ cm}^{-1}$) is

TeO, TeO⁺ (continued):

assumed to correspond to normal atomic products.

^gEstimated (4) from the magnitude of the Ω -type doubling $^h B(1^+) - B(1^-) \approx +0.00066$ (4). | in $X_2 1$ (see ^h).

$i_{D_0^0}(\text{TeO}) + \text{I.P.}(\text{Te}) - \text{I.P.}(\text{TeO})$.

(1) Choong, AP(Paris) (11) 10, 173 (1938).

(2) Haranath, Rao, Sivaramamurty, ZP 155, 507 (1959).

(3) Chandler, Hurst, Barrow, PPS 86, 105 (1965).

(4) Barrow, Hitchings, JP B 5, L132 (1972).

(5) Potts, Williams, CPL 42, 550 (1976).

TeS: See p. 641.

TeSe: See p. 637.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{232}\text{Th}^{(11)}\text{B}$		($\mu = 10.5106174$)		$D_0^0 = 3.0_3 \text{ eV}^a$						JUN 1975
$^{232}\text{Th}^{14}\text{N}$		$\mu = 13.2061097_7$		$D_0^0 = 5.9_0 \text{ eV}^a$						JUN 1975
$^{232}\text{Th}^{16}\text{O}$		$\mu = 14.9634501_8$		$D_0^0 = 9.00 \text{ eV}^a$						JUN 1975
		A good reproduction of the arc spectrum from 11400 to 27800 cm^{-1} can be found in (1).								
		Sequence of R shaded bands; no analysis.								
								R 24291	H	(1)*
K $^1\Pi$	22683.4 ₈	[795.47]	Z (2.30)	$0.318636_{\text{ce}}^{\text{ce}}$ 0.318642_{de}	0.00124_4 0.00132_5^f	$[2.007]$ $[2.025]$	1.88033	K→X,	R 22635.65 Z	(4)
M $^1\Pi$	21752.2	861.41	Z 5.27	$0.325857_{\text{ce}}^{\text{ce}}$ 0.325754_{de}	0.001390^f 0.001398^g	$[2.059]^f$ $[2.051]^g$	1.8595 ₃	M→X,	R 21734.32 Z	(4)*
								R 21407	H	(1)*
		Sequence of R shaded bands; no analysis.								
I $^1\Pi$	19586.29	800.85	Z 1.47	$0.330434_{\text{ch}}^{\text{ch}}$ 0.328921_{dh}	0.001825^i 0.001906^j	2.360^i 2.218^j	1.848 ₆	I→X,	R 19539.06 Z	(3)* (6)
F $^1\Sigma^{(+)}$	(18406)	[757.36] ^k	Z	[0.321397]	^k	[2.042] ^k	[1.87224]	F→X,	R 18337.56 Z	(2)
G $(^1\Delta)^{\ell}$	18038 ^m	816	2.4	0.318192^h	0.00127 ₆	[1.936]	1.88165	G→H,	R 12693.35 Z	(2)* (3)* (6)
E $^1\Sigma^{(+)}$	16353.60 ₈	829.26	Z 2.30	0.323090	0.001303	[1.990]	1.86733	E→X,	R 16320.37 Z	(2)(6)
D $^1\Pi$	15974.5 ₃	[834.22]	Z (2.49)	0.325691^d 0.321549^c	0.001357 0.001298	$[1.997]$ $[1.850]$	1.866	D→X,	R 15946.22 Z	(2)(6)
		Strong unidentified head at 15606 cm^{-1} .								
								R		(1)*
C $^1\Pi$	14520.3 ₅	[830.33]	Z (2.39)	0.322455^c 0.321617^d	0.001281 0.00128_7	$[1.931]$ $[1.873]$	1.870 ₄	C→X,	R 14490.02 Z	(2)(6)
		Violet degraded bands in the region 13700 - 14100 cm^{-1} . No analysis.								
								V		(1)*
B $(^1\Pi)^{\ell}$	11155.57	842.80	Z 2.18	0.324973^c 0.32364^d	0.001299 0.00129	$[1.942]$ $[1.882]$	1.863 ₈	B→X,	R 11129.14 Z	(2)* (6)(7)
A $(^1\Sigma^{+})^{\ell}$	10625.5 ₄	[841.48]	Z (2.44)	0.323044	0.001294	[1.866]	1.86746	A→X,	R 10600.82 Z	(2)* (6)
H $(^1\Phi)^{\ell}$	5321	(864)	(2.4)	0.326427	0.00125 ₈	[1.864]	1.85776			
X $^1\Sigma^{(+)}$	0	895.77	Z 2.39	0.332644	0.001302	[1.833]	1.84032	IR spectrum ⁿ		(9)

ThB: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, HTS 1, 258 (1969).

ThN: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, JCP 49, 19 (1968).

ThO: ^aThermochemical value (mass-spectrom.)(8). (11) prefer
 8.7₉ eV, the difference being largely due to the choice
^bBy electron impact (10)(11). | of free energy functions.
^ce levels.
^df levels.
^ev=0 and 1 of K are perturbed by v=1 and 2 of M, respec-
 tively. The constants given are deperturbed values. An
 unidentified third state interacts strongly with M (4).
^fB₂ = 0.32174; D₁ = 2.178 x 10⁻⁷, D₂ = 3.02 x 10⁻⁷.
^gB₂ = 0.32218; D₁ = 2.026 x 10⁻⁷, D₂ = 2.22 x 10⁻⁷.
^hPerturbations in v=0,1,2,... of I by v=2,3,4,... of G,
 respectively. All constants are deperturbed values.
ⁱγ_e = +0.000106; β_e = +0.055 x 10⁻⁷.
^jγ_e = +0.000063; β_e = -0.015 x 10⁻⁷.

TeS (Table p. 638):

- ^aEstimated (2) by comparison with other molecules of
 this type.
^bInterpretation by (4).
^cOnly one band observed; its isotope shift indicates a
 fairly high value of v'.
^dLong extrapolation from high vibrational levels; only
 v=7,8 of B O⁺ [ΔG(7½) = 196.39] and v=11...15 of A O⁺
 have been analyzed. The v numbering derives from isotope
 shifts of levels which are often perturbed.
^ex ≥ 1084 according to the interpretation by (4) of the

ThO (continued):

- ^kF¹Σ is perturbed; B₁ = 0.324261, D₁ = 3.20₅ x 10⁻⁷.
^lAccording to (5) these states should be identified as
 H ³Δ₁, A ³Π₀⁺, B ³Π₁, G ³Φ₂.
^mFrom the analysis of perturbations; see ^h.
ⁿIn Ar matrix at 15 K.
- (1) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
 - (2) Edvinsson, Selin, Åslund, AF 30, 283 (1965).
 - (3) Edvinsson, von Bornstedt, Nylén, AF 38, 193 (1968).
 - (4) von Bornstedt, Edvinsson, PS 2, 205 (1970).
 - (5) Edvinsson, Thesis (Stockholm, 1971). USIP Report 71-09.
 - (6) Wentink, Spindler, JQSRT 12, 1569 (1972).
 - (7) Zare, Schmeltekopf, Harrop, Albritton, JMS 46, 37
 (1973).
 - (8) Ackermann, Rauh, HTS 5, 463 (1973); JCP 60, 2266 (1974).
 - (9) Gabelnick, Reedy, Chasanov, JCP 60, 1167 (1974).
 - (10) Rauh, Ackermann, JCP 60, 1396 (1974).
 - (11) Hildenbrand, Murad, JCP 61, 1232 (1974).

TeS (continued):

- V shaded UV absorption bands.
^fΔG(½) = 468.04.
^g(3) give B_e = 0.13220, α_e = 0.000545 which do, however, not
 reproduce B₀ and B₁ as determined by them.
- (1) Mohan, Majumdar, PPS 77, 147 (1961).
 - (2) Drowart, Goldfinger, QR 20, 545 (1966).
 - (3) Barrow, Dudley, Hitchings, Yee, JP B 5, L172 (1972).
 - (4) Barrow, Yee, APH 35, 239 (1974).

ThP: ^aThermochemical value (mass-spectrom.)(1).
(1) Gingerich, HTS 1, 258 (1969).

Ti₂: ^aThermochemical value (mass-spectrom.)(1).
(1) Kant, Lin, JCP 51, 1644 (1969).

TiBr: (1) Chatalic, Deschamps, Pannetier, JCPPB 67, 316 (1970).
(2) Sivaji, Rao, JP B 3, 720 (1970).

TiCl: (1) More, Parker, PR 52, 1150 (1937).
(2) Rao, IJP 23, 535 (1949).
(3) Shenyavskaya, Kuzyakov, Tatevskii, OS(Engl. Transl.) 12, 197 (1962).
(4) Parkinson, Reeves, unpublished; quoted by Nicholls, Parkinson, Reeves, AO 2, 919 (1963).
(5) Chatalic, Deschamps, Pannetier, CR C 268, 1111 (1969).
(6) Diebner, Kay, JCP 51, 3547 (1969).
(7) Dunn, Lanini, work reported in progress in Newsletter No. 78 [ed. Phillips, Davis, U. of California (Berkeley, March 1972)].

TiF: ^aEstimated from thermochemical data (1).

(1) Zmbov, Margrave, JPC 71, 2893 (1967).
(2) See ref. (6) of TiCl.
(3) Chatalic, Deschamps, Pannetier, CR C 270, 146 (1970).

Ti¹H, Ti²H:

^aTheoretical predictions of (2).

^bPartial rotational analyses (3) of two V shaded subbands of Ti¹H with P heads at 18576 and 18646 cm⁻¹ give the lower state constants B" = 4.956 and 5.22, respectively. The upper states are strongly perturbed. The bands have P, Q, and R branches.

^cDiffuse.

(1) Smith, Gaydon, JP B 4, 797 (1971).
(2) Scott, Richards, JP B 7, 500 (1974).
(3) Gaydon, JP B 7, 2429 (1974).

TiI: (1) Sivaji, Rao, Rao, CS 39, 153 (1970).

TiO (continued from p. 647):

(54) Rauh, Ackermann, JCP 60, 1396 (1974).
(55) Collins, JP B 8, 304 (1975).
(56) Żyrnicki, JQSRT 15, 575 (1975).
(57) Liu, Wahlbeck, JCP 63, 1694 (1975).
(58) Brom, Broida, JCP 63, 3718 (1975).
(59) Feinberg, Bilal, Davis, Phillips, ApL 12, 147 (1976);
Feinberg, Davis, JMS 65, 264 (1977).

(60) Hildenbrand, CPL 44, 281 (1976).
(61) Dubois, Gole, JCP 66, 779 (1977).
(62) Linton, Broida, JMS 64, 382, 389 (1977).
(63) Sheldon, Gilles, JCP 66, 3705 (1977);
Wheatley, Sheldon, Gilles, JCP 66, 3712 (1977).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{48}\text{Ti}^{14}\text{N}$		$\mu = 10.8378951_7$ $D_0^0 = 4.9 \text{ eV}^a$ Additional bands in the region $30400 - 33800 \text{ cm}^{-1}$; in absorption and in emission.								MAY 1976
B $^2\Sigma$								B \rightarrow X, R	23487.3 Z	(1)
A $^2\Pi_r$	b	c						A \rightarrow X, R	16197.25 ^e Z	(6)
X $^2\Sigma$	0	c								(4)*
$(^{48})\text{Ti}^{16}\text{O}$		$(\mu = 11.9938851_9)$ $D_0^0 = 6.87 \text{ eV}^a$ I.P. = 6.4 eV^b Very weak progression ($\omega_e'' \approx 994$, $\omega_e'' x_e'' \approx 5$) of R shaded bands in emission from flames.								NOV 1977 A
D	(31920)	[(1040)]						D \leftrightarrow X, ^c	(30422) (30367) (31940)	H H (34)(44) (34)(36)(44) (61)
e $^1\Sigma^+$	a+26598.1	[845.2]	Z 4.2 H	0.4892 ^d	0.0023	[4.7] ^d	1.695 ₀	e \leftrightarrow d, R	24297.5 Z	(37)* (42)* (52)
f $^1\Delta$	a+(19132)	(890)		[0.50221]		[6.4]	[1.6729 ₂]	f \leftrightarrow a, ^e R	19068.93 Z	(43)* (52)
c $^1\phi$	a+17890.2	[909.6]	Z 4.1 ₉ H	0.5230 ^f	0.0031 ₃	[3.9] ^f	1.639 ₃	c \leftrightarrow a, ^{eh} R β bands	17840.6 Z	(3)(6)* (14)* (29) (33)(41)(51) (2)* (4)(9) (11)(14)*
C $^3\Delta_r$	19617.0 19525.5 19427.12	838.26	Z 4.76 ⁱ	0.48989 ^{jk}	0.00306 ^l	6.7	1.6938 ₃	C \leftrightarrow X, ^{mn} R α bands	19334.03 Z 19343.66 Z 19341.68 Z	(20)(21)(31) (33)(45)(48) (49)
B $^3\Pi_r$	16331.3 16315.1 16293.5	875	H 5	[0.50617] ^{jp}		[6.86]	[1.6663 ₆]	C \rightarrow a, ^o		(62)
b $^1\Pi$	a+11322.0 ₃	[911.20]	Z (3.7 ₂)	0.51337 ^r	0.0029 ₁	6.1	1.6546 ₄	B \leftrightarrow X, ^m R γ' bands	16066.7 ^q Z 16151.6 ^q Z 16226.4 Z	(5)(14)* (17)(18)(24) (31)* (38)* (48)(55)
								b \leftrightarrow d, ^e R ϕ bands	9054.02 Z	(15)(19)(29) (30)(33)(49) (52)(58)
								b \leftrightarrow a, ^e R δ bands	11272.82 Z	(6)* (29)(30) (33)(52)(58)
								(b \rightarrow X), ^s	(14710)	(58)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(48) Ti^{16}O (continued)										
A $3\phi_r$	14431.0 14262.8 14089.91	867.78	Z 3.942	0.50739 ^j	0.00315 ^t	6.92 ^t	1.6643 ₆	A \leftrightarrow X, mn R γ bands	14163.00 Z 14095.88 Z 14019.43 Z	(1)(3)(7)* (10)(11) (14)* (21) (31)(48)(49)
E 3Π	12025	924.2	H 5.1					E \leftrightarrow X, u ϵ bands	11871 H 11886 H 11899 H	(36)(62)
d $1\Sigma^+$	a + 2215.6	[1014.6]	Z (4.6 ₄)	0.54922	0.00337	[6.0]	1.5997 ₂			
a 1Δ	a ^v	[1009.3]	H 3.9 ₃	0.53760	0.00298	5.9	1.6169 ₂			
X $3\Delta_r$	197.5 ^w 96.4 ^w 0	1009.02	Z 4.498 ^x	0.53541 ^j	0.00301 ^y	6.03 ^y	1.6202 ₂	Rotation-vibr. sp. ^z		

TiN: ^aThermochemical value (mass-spectrom.)(5). See also
^b $A_0 = +156.70$; slight J dependence. | (2)(3).

^c0-0 sequence only; the R_2+Q_{21} and Q_1+R_{12} heads of the
0-0 band are at 16285.8 and 16125.8 cm^{-1} , the corres-
ponding heads of the 1-1 band at 16193.2 and 16035.2.

^d Λ -type doubling in $2\Pi_{1/2}$, $\Delta v = 0.037(J+\frac{1}{2})$. Perturbations.

^eRefers to the zero-point of the Hill-Van Vleck expres-
sion in the upper state. (4) give 16197.52, in poor
agreement with our recalculated value 16197.21. We as-
sume that the former is intended to be 16197.25.

- (1) Parkinson, Reeves, CJP 41, 702 (1963).
- (2) Carlson, Claydon, Moser, JCP 46, 4963 (1967).
- (3) Gingerich, JCP 49, 19 (1968).
- (4) Dunn, Hanson, Rubinson, CJP 48, 1657 (1970).
- (5) Stearns, Kohl, HTS 2, 146 (1970).
- (6) Bates, Ranieri, Dunn, CJP 54, 915 (1976).

TiO: ^aThermochemical value (mass-spectrom.)(27)(35)(57)(60);
different values have been proposed by (26)(28)(40). See
also (12)(13)(47)(63). A lower bound of 6.9₃ eV for the
dissociation energy has been deduced by (61) from the
study of chemiluminescent spectra resulting from the re-
actions $\text{Ti} + \text{O}_2$ and $\text{Ti} + \text{N}_2\text{O}$.

^bElectron impact appearance potential (54).

^cMultiple heads in flames. Absorption in a neon matrix at
4 K. Analysis uncertain.

^dPerturbations in $v=0$ and 1 by levels of smaller B values
(52). $D_1 = 9.1 \times 10^{-7}$.

^eAbsorption in stellar atmospheres.

^fThe data suggest a slight perturbation of $v=0$ by an un-
identified level of smaller B value and lower energy.
 $D_1 \dots D_3 (10^{-7} \text{ cm}^{-1}) = 5.8, 6.9, 7.5$; $H_0 = -2.3 \times 10^{-11}$.

^gRadiative lifetime $\tau(v=0) = 17.5 \text{ ns}$ (59). See ^h.

^hThe absolute transition probabilities of (56) are in gross
(continued p. 646)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions Design. v_{00}	References
(48)Ti ³² S		$(\mu = 19.1816179) \quad D_0^0 = 4.7_5 \text{ eV}^a$							JUN 1975
C $^3\Delta$	$\begin{cases} 3 & (11806) \\ 2 & (11716) \\ 1 & 11624.3 \end{cases}$	484.12	Z 2.55	0.18905	0.00102 ^b	[1.22]	2.1610	C \leftrightarrow X, R 11582.25 Z 11587.05 Z 11585.31 Z	(4)
		484.30	Z 2.51 ₅	0.18820 ^c	0.00099 ^d	[1.20]			
				[0.18684]	e	[1.06]			
(X) $^3\Delta$	$\begin{cases} 3 & (185)^f \\ 2 & (90)^f \\ 1 & 0 \end{cases}$	[558.17]	Z	0.20344	0.00092	[1.12]	2.0825		
		[558.30]	Z (1.95)	0.20268	0.00092	[1.09 ₅]			
		[558.37]	Z	0.20180	0.00090	[1.03 ₅]			
(48)Ti (¹³⁰)Te		$(\mu = 35.021596_7) \quad D_0^0 = 2.94 \text{ eV}^a$							JUN 1975

TiS: ^aThermochemical value (mass-spectrom.)(3); see also (1)

^b $\gamma_e = -0.00001_3$. | [quoted in (2)].

^cSmall perturbations in $v=0$.

^d $\gamma_e = -0.00001_9$.

^eExtensive perturbations.

^fEstimated from the effective B values.

(1) Franzen, Thesis (U. of Kansas, 1962).

TiS (continued):

(2) Suzuki, Wahlbeck, JPC 70, 1914 (1966).

(3) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

(4) Clements, Barrow, TFS 65, 1163 (1969).

TiTe: ^aThermochemical value (mass-spectrom.)(1); no details.

(1) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

TiO (continued):

disagreement with the lifetime measurements of (59).

ⁱ $w_e \gamma_e = +0.047$.

^jFor spin coupling constants (spin-orbit, spin-spin, spin-rotation) see (48), also (23)(25)(32).

^kLevels with $v \geq 4$ are perturbed (45)(48). The perturbing (singlet?) state has $B \approx 0.510$, $w \approx 900$.

^l $\gamma_e = -0.000030$.

^mAbsorption in stellar atmospheres. Also observed in absorption in rare gas matrices (24)(36).

TiO (continued):

ⁿElectronic oscillator strengths for the α system (39)(50), for the γ bands (39).

^oOnly three lines [R(16), Q(17), P(18)] of the $^3\Delta_3 \rightarrow ^1\Delta$ 2-0 band have been observed in laser-excited photoluminescence.

^pThe Λ -type doubling in $^3\Pi_0$, $\Delta v = 1.60 \text{ cm}^{-1}$, is nearly constant up to $J \approx 65$, then diminishes and changes sign for

$q_{v_{00}}(^3\Pi_1 - ^3\Delta_1) = 16248.0$, $v_{00}(^3\Pi_2 - ^3\Delta_2) = 16167.8$. | $J > 120$.

^r Λ -type doubling $\Delta v_{fe} = +0.00014 J(J+1)$.

^sIn neon at 4 K.

TiO (continued):

$$^t\gamma_e = -0.000010; \beta_e = +0.02 \times 10^{-7}.$$

^uAbsorption in a neon matrix at 4 K.

^v $a = 3440 \pm 10 \text{ cm}^{-1}$ (62), based on the identification of three lines of the C→a 2-0 band (see ^o). A similar value ($a \approx 3500$) follows from the assignment (58) of the b→X intercombination transition in neon. Qualitative agreement with theoretical predictions (22). Earlier estimates (8)(18) are considerably lower.

^wFrom the observation of two satellite bands of $\gamma'(0-0)$ (38); see ^q.

$$^xw_e y_e = -0.0107.$$

$$^y\gamma_e = -0.000011; \beta_e = +0.03 \times 10^{-7}.$$

^zNot observed; for the predicted structure of the fundamental band see (53).

- (1) Christy, ApJ 70, 1 (1929).
- (2) Christy, PR 33, 701 (1929).
- (3) Lowater, PPS 41, 557 (1929).
- (4) Budó, ZP 28, 437 (1936).
- (5) Coheur, BSRSL 12, 98 (1943).
- (6) Phillips, ApJ 111, 314 (1950).
- (7) Phillips, ApJ 114, 152 (1951).
- (8) Phillips, ApJ 115, 567 (1952).
- (9) Phillips, ApJ 119, 274 (1954).
- (10) Fraser, Jarman, Nicholls, ApJ 119, 286 (1954).
- (11) Uhler, Dissertation (Stockholm, 1954).
- (12) Groves, Hoch, Johnston, JPC 52, 127 (1955).
- (13) Berkowitz, Chupka, Inghram, JPC 61, 1569 (1957).
- (14) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (15) Pettersson, AF 16, 185 (1959).
- (16) Ortenberg, OS(Engl. Transl.) 2, 80 (1960).
- (17) Pedoussaut, CR 252, 2819 (1961).
- (18) Merrill, Deutsch, Keenan, ApJ 136, 21 (1962).
- (19) Pettersson, Lindgren, AF 22, 491 (1962).
- (20) Prasad, PPS 79, 1078 (1962); 82, 419 (1963).

TiO (continued):

- (21) Ortenberg, Glasko, SAAJ 6, 714 (1963).
- (22) Carlson, Nesbet, JCP 41, 1051 (1964); Carlson, Moser, JCP 46, 35 (1967).
- (23) Kovács, JMS 18, 229 (1965).
- (24) Weltner, McLeod, JPC 69, 3488 (1965).
- (25) Törös, APH 20, 91 (1966).
- (26) Wahlbeck, Gilles, JCP 46, 2465 (1967).
- (27) Drowart, Coppens, Smoes, JCP 50, 1046 (1969).
- (28) Gilles, Hampson, Wahlbeck, JCP 50, 1048 (1969).
- (29) Linton, Nicholls, JP B 2, 490 (1969).
- (30) Lockwood, ApJ 157, 275 (1969).
- (31) Phillips, ApJ 157, 449 (1969).
- (32) Kovács, Korwar, APH 29, 399 (1970).
- (33) Linton, Nicholls, JQSRT 10, 311 (1970).
- (34) Pathak, Palmer, JMS 33, 137 (1970).
- (35) Hampson, Gilles, JCP 55, 3712 (1971).
- (36) McIntyre, Thompson, Weltner, JPC 75, 3243 (1971).
- (37) Phillips, Davis, ApJ 167, 209 (1971).
- (38) Phillips, ApJ 169, 185 (1971).
- (39) Price, Sulzmann, Penner, JQSRT 11, 427 (1971); 14, 1273 (1974).
- (40) Balducci, De Maria, Guido, Piacente, JCP 56, 3422 (1972).
- (41) Dube, IJPAP 10, 70 (1972).
- (42) Lindgren, JMS 43, 474 (1972).
- (43) Linton, CJP 50, 312 (1972).
- (44) Palmer, Hsu, JMS 43, 320 (1972).
- (45) Phillips, Davis, ApJ 175, 583 (1972).
- (46) Wentink, Spindler, JQSRT 12, 1569 (1972).
- (47) Wu, Wahlbeck, JCP 56, 4534 (1972).
- (48) Phillips, ApJ(Suppl.) 26 (232), 313 (1973).
- (49) Collins, Fay, JQSRT 14, 1259 (1974).
- (50) Fairbairn, Wolnik, Berthel, ApJ 193, 273 (1974).
- (51) Linton, JMS 50, 235 (1974).
- (52) Linton, Singhal, JMS 51, 194 (1974).
- (53) Phillips, ApJ(Suppl.) 27 (247), 319 (1974).

(continued p. 643)

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-9} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(205) Tl_2		($\mu = 102.487219$)	$D_0^0 < 0.9 \text{ eV}^a$ Several diffuse emission bands and continua, 15000 - 36500 cm^{-1} . Strong R and V shaded absorption bands, 22900 - 23500 cm^{-1} . Weak R shaded bands in thermal emission, 15000 - 16000 cm^{-1} . $\omega' \approx 88$, $\omega'' \approx 136 \text{ cm}^{-1}$.						NOV 1977 (1) (3) (3)	
(205) Tl^{40}Ar		($\mu = 33.4423676$)	The far-wing emission intensities of the Tl resonance lines (26478 and 18685 cm^{-1}) broadened by rare gases, have been studied by (1); Franck-Condon analyses of the observed continua yield potential curves in the 3-4 \AA region for the $X_1 \frac{1}{2}$, $X_2 \frac{3}{2}$, $A \frac{1}{2}$, $B \frac{2}{2}$ states arising from the atomic limits $^2P_{\frac{1}{2}}$, $^2P_{\frac{3}{2}}$, $^2S_{\frac{1}{2}}$ + 1S . Near-wing intensities have been investigated by (2) yielding additional information on the potentials at larger internuclear distances.						NOV 1977	
(205) Tl^{75}As		($\mu = 54.866846_3$)	$D_0^0 = 2.0_2 \text{ eV}^a$						NOV 1977	
(205) Tl^{209}Bi		($\mu = 103.479018$)	$D_0^0 = 1.2_1 \text{ eV}^a$						NOV 1977	
$^{205}\text{Tl}^{81}\text{Br}$		$\mu = 58.014373$	$D_0^0 = 3.42 \text{ eV}^a$ I.P. = 9.14 eV^b Fragments of an emission system at $\sim 25340 \text{ cm}^{-1}$. Continuous absorption for $v > 40000 \text{ cm}^{-1}$. Continuous absorption with maximum at 37160 cm^{-1} . ^d Weak absorption continua at 31000 and 32040 cm^{-1} . Absorption continua with maxima at 29540 and 30000 cm^{-1} . ^d 108.32 H 5.15 ^f Bands having $v' \geq 3$ are diffuse.						NOV 1977 (2)* (4)* (2)(11) (1)(2)(11)* (11)* (1)* (2)(11)* (1)* (2)* (3)(4) (13) (5)(6)(16) (12)	
D								(D→A), R		
C ($^1\Pi$)								C←X, ^c ^c ^c		
A ($^3\Pi_0$) ^e	29191.5							A↔X, ^c R 29148.4 H		
X $^1\Sigma^+$	0	192.10 H	0.39	0.0423895 ^g	0.0001275 ₅	(8.3)	2.61819 ₁	IR spectrum ^h Microwave sp. ⁱ Mol. beam el. reson. ^j		

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(205)Tl(79)Br ⁺										
						$D_0^0 = 0.39 \text{ eV}^k$				NOV 1977
B $^2\Sigma$	(36500)	}	From the photoelectron spectrum (15), using vertical potentials for A and B and the adiabatic potential for X $^2\Pi$. The peak corresponding to the shallow $^2\Pi$ state is very broad and has a vertical potential which lies at $\sim 0.35 \text{ eV}$ above that of A $^2\Sigma$.							
A $^2\Sigma$	(2700)									
X $^2\Pi$	0									

Tl₂: ^aMass-spectrometric result of (2) who suggest the "pre-ferred" value 0.6 eV.

(1) Hamada, PM 12, 50 (1931).

(2) Drowart, Honig, JPC 61, 980 (1957).

(3) Ginter, Ginter, Innes, JPC 69, 2480 (1965).

TlAr: (1) Cheron, Scheps, Gallagher, JCP 65, 326 (1976).

(2) Cheron, Scheps, Gallagher, PR A 15, 651 (1977).

TlAs: ^aThermochemical value (mass-spectrom.)(1).

(1) Piacente, Malaspina, JCP 56, 1780 (1972).

TlBi: ^aThermochemical value (mass-spectrom.)(1).

(1) De Maria, Malaspina, Piacente, JCP 56, 1978 (1972).

TlBr, TlBr⁺:

^aPhotoionization mass-spectrometry (10). In good agreement with spectroscopic and thermochemical results (7), flame photometry (8), and electron impact mass-spectrometry (9).

^bPhotoionization value (10). Notice that this is the adiabatic value corresponding to the second vertical potential (9.83 eV) observed in the photoelectron spectrum (15); first vertical I.P. at 9.48 eV.

^cAbsorption cross sections have been measured by (11).

TlBr, TlBr⁺ (continued):

^d(2) report emission continua with maxima at 30020 and 33770

^eAssigned by analogy with TlCl; (2) assume $^3\Pi_1$. | cm^{-1} .

^f $w_e y_e = -0.22$.

^g(16) give rotational constants for four isotopes.

^hIn argon at 10 K.

ⁱDipole moment of $^{205}\text{Tl}^{79}\text{Br}$; $\mu_{el}(v=0) = 4.49 \text{ D}$, from Stark effect of rotation sp. (14).

^jHfs constants for four isotopes in the first five vibra-

^k $D_0^0(\text{TlBr}) + \text{I.P.}(\text{Tl}) - \text{I.P.}(\text{TlBr})$. | tional states.

(1) Butkow, ZP 58, 232 (1929).

(2) Howell, Coulson, PPS 53, 706 (1941).

(3) Rao, IJP 23, 265 (1949).

(4) Rao, IJP 23, 425 (1949).

(5) Barrett, Mandel, PR 109, 1572 (1958).

(6) Fitzky, ZP 151, 351 (1958).

(7) Barrow, TFS 56, 952 (1960).

(8) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(9) Khvostenko, Sultanov, RJPC 39, 252 (1965).

(10) Berkowitz, Walter, JCP 49, 1184 (1968).

(11) Davidovits, Bellisio, JCP 50, 3560 (1969).

(continued p. 651)

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{205}\text{Tl}^{35}\text{Cl}$										
D		$\mu = 29.8725631$ $D_0^0 = 3.82 \text{ eV}^a$ I.P. = 9.70 eV^b							NOV 1977	
C ($^1\Pi$)		Complex system of emission bands; tentative vibrational analysis (3). Continuous absorption for $\nu > 40000 \text{ cm}^{-1}$. Continuous absorption with maximum at 39820 cm^{-1} , preceded by diffuse bands of longer wavelengths. Very weak absorption continua with maxima at 32910 and 34830 cm^{-1} . Absorption continua with maxima at 31690 and 32190 cm^{-1} .						(D \rightarrow A), R_V $\begin{smallmatrix} (24628) \\ (24040) \end{smallmatrix}$	(2)* (3)* (1)(16)	
A $^3\Pi_0^+$	31049.4	223.1 ^d (Z)	11.4 ^e	0.09227 ₀ ^f	0.00131	0.7 ₅	2.4730	C \leftarrow X, $\begin{smallmatrix} c \\ c \\ c \end{smallmatrix}$	(1)* (16)* (1)* (16)* (1)* (16)*	
X $^1\Sigma^+$	0	283.7 ₅ ^d (Z)	0.81 ₈	0.09139702 ₂	0.00039793 ₂ ^g	0.375 ₃	2.484826	A \leftrightarrow X, $\begin{smallmatrix} c \\ c \end{smallmatrix}$ R 31016.6 (Z)	(1)* (2)* (6)	
								Vibration sp. ^h	(17)(21)	
								Rotation sp.	(7)(8)(12) (20)	
								Mol. beam electric and magnetic resonance ⁱ	(4)(15)(19) (5)	
$(^{205}\text{Tl}^{35}\text{Cl})^+$										
B $^2\Sigma$	(33800)	$D_0^0 = 0.23 \text{ eV}^j$							NOV 1977	
A $^2\Sigma$	(1600)	From the photoelectron spectrum (18), using vertical potentials for A and B and the adiabatic potential for X. The $^2\Pi$ peak is very broad and has a vertical potential which is 0.49 eV higher than that of A $^2\Sigma$.								
X $^2\Pi$	0									
$^{205}\text{Tl}^{19}\text{F}$										
		$\mu = 17.3868727$ $D_0^0 = 4.57 \text{ eV}^a$ I.P. = 10.52 eV^b							NOV 1977	
C ($^1\Pi$)	(45546)	(2) report emission bands in the region $28500 - 29500 \text{ cm}^{-1}$; uncertain. Absorption continua at ~ 45400 and above 50000 cm^{-1} . [346] H Only $\nu=0$ and 1 . ^c						C \leftarrow X, R 45481 H	(1)* (1)* (1)*	
B $^3\Pi_1$	36863.0 ₈	366.6 ₄	10.2 ₂ ^{de}	0.2249 ₂	0.0030 ₇ ^f	[3.9] ₂ ^g	2.076 ₂	B \leftrightarrow X, R 36805.6 ₃ Z	(1)* (3)	
A $^3\Pi_0^+$	35186.0 ₂	436.3	7.1 ^{he}	0.2309 ₁	0.0027 ₄ ⁱ	2.8 ₁ ^j	2.049 ₁	A \leftrightarrow X, V_R 35164.3 ₁ Z	(1)* (3)	
X $^1\Sigma^+$	0	477.3	2.3	0.223150163	0.001503850 ^k	1.948	2.084438	Vibration sp. ^l	(16)(21)	
								Rotation sp.	(12)(15)(17) (19)(20)	
								Mol. beam el. reson. ^m	(6)(7)(10) (11)	

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
(205) Tl^{19}F^+		$D_0^0 = 0.16 \text{ eV}^n$								NOV 1977	
B	$^2\Sigma$	(28500)	} From the photoelectron spectrum (18) (adiabatic potentials). The peak corresponding to A is very broad.								
A	$^2\Pi$	(5100)									
X	$^2\Sigma$	0									

TlBr , TlBr^+ (continued):

- (12) Dickinson, Stephenson, Zorn, JCP 53, 1525 (1970).
- (13) Brom, Franzen, JCP 54, 2874 (1971).
- (14) Tiemann, ZN 26 a, 1809 (1971).
- (15) Berkowitz, JCP 56, 2766 (1972).
- (16) Lovas, Tiemann, JPCRD 3(3), 609 (1974).

TlCl , TlCl^+ :

^aPhotoionization mass-spectrometry (14); good agreement with thermochemical and spectroscopic values (9)(10), electron impact mass-spectrometry (13), and flame photometry (11).

^bPhotoionization value (14). As for TlBr , this adiabatic potential corresponds to the second rather than first vertical potential observed by photoelectron spectroscopy (18).

^cAbsorption cross sections (16).

^dVibrational constants of (2) whose measurements at higher dispersion are more extensive than those of (1). Rotational analyses (6) give $\Delta G'(\frac{1}{2}) = 201.60$, $\Delta G''(\frac{1}{2}) = 281.88$.
 $w_e v_e = +1.33$, $w_e z_e = -0.115$.

^fPredissociation for $v' \geq 4$; see (2).

$\bar{\epsilon}_{0e} = +4.17_0 \times 10^{-7}$; from (12) who gives rotational constants for all four TlCl isotopes. See also (20).

TlCl , TlCl^+ (continued):

^hIR and Raman spectra in argon and krypton matrices.

ⁱ $\mu_{el} = 4.515_3 + 0.0552_7(v + \frac{1}{2}) + 0.00007_8(v + \frac{1}{2})^2 \text{ D}$; from (19) who give also hfs constants and magnetic parameters for $J_{D_0^0}(\text{TlCl}) + \text{I.P.}(\text{Tl}) - \text{I.P.}(\text{TlCl})$.
 $v = 0 \dots 3$.

- (1) Howell, Coulson, PRS A 166, 238 (1938).
- (2) Miescher, HPA 14, 148 (1941).
- (3) Rao, IJP 23, 393 (1949).
- (4) Carlson, Lee, Fabricand, PR 85, 784 (1952).
- (5) Zeiger, Bolef, PR 85, 788 (1952).
- (6) Barrow, PPS A 70, 622 (1957).
- (7) Barrett, Mandel, PR 109, 1572 (1958).
- (8) Fitzky, ZP 151, 351 (1958).
- (9) Barrow, PPS 75, 933 (1960).
- (10) Barrow, TFS 56, 952 (1960).
- (11) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (12) De Wijn, Physica 31, 1193, 1557 (1965).
- (13) Khovstenko, Sultanov, RJPC 39, 252 (1965).
- (14) Berkowitz, Walter, JCP 49, 1184 (1968).
- (15) Hammerle, Dickinson, VanAusdal, Stephenson, Zorn, JCP 50, 2086 (1969).

(continued p. 653)

TlF , TlF^+ : See p. 653.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
(205) Tl^1H		$(\mu = 1.00289416) \quad D_0^0 = 1.97 \text{ eV}^a$ Absorption continua at 22720, 23590, 23920, 24550, 24930 cm^{-1} .								NOV 1977
D $3\Pi_2$ (2) [24344.3]				[1.53] ^b		[35]	[3.31]	C \leftarrow X, R	23654.6 Z	(3)
C 1Π (1) (24181)		[98.0 ₅] Z	c	[2.027] ^d	e	[27] ^f	[2.880]	D \leftarrow X, R	23556.25 Z	(4)
B $3\Pi_1$ (1)		Unstable.								(4)*
A $3\Pi_0+(0^+)$ (17723)		[759.1] Z	gh	[4.617]	hij	[5.6 ₈] ^k	[1.908 ₁]	A \leftrightarrow X, R	17519.9 Z	(1)* (3)
X $1\Sigma^+$ 0		1390.7 Z	22.7	4.806 ^l	0.154 ^m	[2.54]	1.870 ₂			
(205) Tl^2H		$(\mu = 1.99450400) \quad D_0^0 = 2.00 \text{ eV}^n$								NOV 1977
C 1Π (1)		$\Delta G(3/2) = 57.56$		$B_2 = 0.820$ $B_1 = 0.973$		$D_2 = 16$ $D_1 = 11$	$r_1 = 2.94_7$	D \leftarrow X, ^o R	$v(1-0) = 23823.69$ Z	(6)
A $3\Pi_0+(0^+)$ (17717)		[604.50] Z	ph	[2.380]	hqj	[1.14] ^k	[1.884 ₅]	A \leftarrow X R	17590.21 Z	(3)*
X $1\Sigma^+$ 0		987.7 Z	12.04 ^r	2.419	0.057 ^s	0.60	1.869 ₂			

 $Tl^1H, Tl^2H:$

^aFrom the highest observed level in C 1Π (4); this state dissociates to $2P_{3/2} + 2S$. Flame photometry (2) gives 1.9₁ eV.

^bThis level interacts with $v=1$ of C 1Π (4).

^c $\Delta G(3/2) = 56.2$.

^d $B_0^+ - B_0^- = +0.006$.

^e $B_1 = 1.84, B_2 = 0.7$.

^f $D_1 = 60 \times 10^{-4}$.

^g $\Delta G(3/2 \dots 11/2) = 474.9, 393.0, 402.2, 416.0, 426.1$.

^hAnomalous potential curve, see (5)(6).

ⁱ $B_1 \dots B_6 = 3.916, 3.201, 2.981, 2.856, 2.780, 2.692$.

^jLines become increasingly diffuse with increasing rotation.

 Tl^1H, Tl^2H (continued):

^kFor higher D_v values see (1)(3).

^lRKR potential curve (5).

^m $y_e = +0.0044$.

ⁿFrom the value for Tl^1H .

^o $v'=0$ not observed, possibly because of predissociation by the repulsive $3\Pi_1$ state; see (6).

^p $\Delta G(3/2 \dots 11/2) = 439.13, 314.61, 279.65, 281.23, 288.14$.

^q $B_1 \dots B_6 = 2.144, 1.842, 1.614, 1.515, 1.47, 1.43$.

^r $w_{ey_e} \approx +0.1$.

^s $y_e = +0.002$.

Tl^1H , Tl^2H (continued):

- (1) Grundström, Valberg, ZP 108, 326 (1938).
- (2) Bulewicz, Sugden, TFS 54, 830 (1958).
- (3) Neuhaus, Muld, ZP 153, 412 (1959).

- (4) Larsson, Neuhaus, AF 23, 461 (1963).
- (5) Ginter, Battino, JCP 42, 3222 (1965).
- (6) Larsson, Neuhaus, AF 31, 299 (1966).

$TlCl$, $TlCl^+$ (continued):

- (16) Davidovits, Bellisio, JCP 50, 3560 (1969).
- (17) Brom, Franzen, JCP 54, 2874 (1971).
- (18) Berkowitz, JCP 56, 2766 (1972).
- (19) Ley, Schauer, ZN 27 a, 77 (1972).
- (20) Lovas, Tiemann, JPCRD 3(3), 609 (1974).
- (21) Lesiecki, Nibler, JCP 63, 3452 (1975).

TlF , TlF^+ (Table p. 650/1):

^aPhotoionization mass-spectrometry (14); good agreement with thermochemical results [(8) and ref. given in (14)]; similar results by equilibrium mass-spectrometry (13) and flame photometry (9).

^bAdiabatic potential from the photoelectron spectrum (18).

^cAccording to (8) [see Table 3, Note c of this reference] the vibrational analysis is uncertain and the 0-0 band may lie at 45010 cm^{-1} .

$$d_{we} = -1.155.$$

^eBoth A and B have small potential humps of $\sim 0.18 \text{ eV}$.

$$f_{ye} = -0.000905.$$

$$g_{D1} = 5.22 \times 10^{-7}, D_2 = 6.73 \times 10^{-7}.$$

$$h_{we} = -0.1.$$

$$i_{ye} = -0.000135.$$

$$j_{\beta} = +0.22 \times 10^{-7}.$$

$$k_{ye} = +3.142 \times 10^{-6} \text{ (17)}.$$

^lIR and Raman spectra in argon and krypton matrices.

TlF , TlF^+ (continued):

$$m_{el} = 4.1936 + 0.0691(v + \frac{1}{2}) D; g_J = -0.05356 \mu_N \text{ (11)}.$$

$$n_{D0}^0(TlF) + I.P.(Tl) - I.P.(TlF).$$

- (1) Howell, PRS A 160, 242 (1937).
- (2) Rao, Rao, IJP 29, 20 (1955).
- (3) Barrow, Cheall, Thomas, Zeeman, PPS 71, 128 (1958).
- (4) Barrett, Mandel, PR 109, 1572 (1958).
- (5) Fitzky, ZP 151, 351 (1958).
- (6) Gräff, Paul, Schlier, ZP 153, 38 (1958).
- (7) Gräff, ZP 155, 433 (1959).
- (8) Barrow, TFS 56, 952 (1960).
- (9) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).
- (10) Drechsler, Gräff, ZP 163, 165 (1961).
- (11) Boeckh, Gräff, Ley, ZP 179, 285 (1964).
- (12) Ritchie, Lew, CJP 43, 1701 (1965).
- (13) Murad, Hildenbrand, Main, JCP 45, 263 (1966).
- (14) Berkowitz, Walter, JCP 49, 1184 (1968).
- (15) Hoeft, Lovas, Tiemann, Törring, ZN 25 a, 1029 (1970).
- (16) Brom, Franzen, JCP 54, 2874 (1971).
- (17) Dijkerman, Flegel, Gräff, Mönster, ZN 27 a, 100 (1972).
- (18) Dehmer, Berkowitz, Cusachs, JCP 58, 5681 (1973).
- (19) Honerjäger, Tischer, ZN 28 a, 458 (1973).
- (20) Lovas, Tiemann, JPCRD 3(3), 609 (1974).
- (21) Lesiecki, Nibler, JCP 63, 3452 (1975).

TlI, TlI⁺:

^aPhotoionization mass-spectrometry (11); similar values are obtained from thermochemical data (9), by flame photometry (10), and by photofragment spectroscopy (18).

^bPhotoionization mass-spectrometry (11) and photo-electron spectroscopy (16).

^cAbsorption cross sections (12).

^d $\Delta G(\frac{1}{2}) = 143.0 \text{ cm}^{-1}$ in argon at 10 K (14).

^e $\mu_{el}(v=0) = 4.61 \text{ D}$, from Stark effect of rotation sp.(15).

^fHfs constants.

$\epsilon_{D_0}^0(\text{TlI}) + \text{I.P.}(\text{Tl}) - \text{I.P.}(\text{TlI})$.

(1) Butkow, Terenin, ZP 49, 865 (1928).

(2) Butkow, ZP 58, 232 (1929).

(3) Rao, Rao, IJP 23, 185 (1949).

(4) Rao, IJP 24, 434 (1950).

(5) Rao, Rao, IJP 29, 20 (1955).

(6) Happ, ZP 147, 567 (1957).

(7) Barrett, Mandel, PR 109, 1572 (1958).

(8) Fitzky, ZP 151, 351 (1958).

(9) Barrow, TFS 56, 952 (1960).

(10) Bulewicz, Phillips, Sugden, TFS 57, 921 (1961).

(11) Berkowitz, Chupka, JCP 45, 1287 (1966).

(12) Davidovits, Bellisio, JCP 50, 3560 (1969).

(13) Stephenson, Dickinson, Zorn, JCP 53, 1529 (1970).

(14) Brom, Franzen, JCP 54, 2874 (1971).

(15) Tiemann, ZN 26 a, 1809 (1971).

(16) Berkowitz, JCP 56, 2766 (1972).

(17) Lovas, Tiemann, JPCRD 3(3), 609 (1974).

(18) Kawasaki, Litvak, Bersohn, JCP 66, 1434 (1977).

Tm0: ^aThermochemical value (mass-spectrom.)(4), recal. (5).
 (1) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
 (2) Herrmann, Alkemade, "Chemical Analysis by Flame Photometry", Wiley-Interscience (1963).
 (3) Mavrodineanu, Boiteux, "Flame Spectroscopy", Wiley (1965).
 (4) Ames, Walsh, White, JPC 71, 2707 (1967).
 (5) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

UB: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, JCP 53, 746 (1970).

UC: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, JCP 50, 2255 (1969).

UN: ^aThermochemical value (mass-spectrom.)(1).
 (1) Gingerich, JCP 47, 2192 (1967).

UO: ^aThermochemical value (mass-spectrom.)(3)(4)(5).
^bElectron impact appearance potential, average of two values (2)(8).
^cIR spectrum of U¹⁶O in Ar matrix at 15 K (6)(7). For U¹⁸O at 776.3 cm⁻¹. Derived constants for U¹⁶O are $\omega_e = 825.0$, $\omega_e x_e = 2.5$.
 (1) See ref. (1) of Tm0.
 (2) Mann, JCP 40, 1632 (1964).
 (3) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).
 (4) Coppens, Smoes, Drowart, TFS 64, 630 (1968).
 (5) Pattoret, Drowart, Smoes, in "Thermodynamics of Nuclear Materials" (Proc. Symp. Thermodynamics, Vienna, 1967), p. 613. Publ. IAEA, Vienna (1968).
 (6) Carstens, Gruen, Kozlowski, HTS 4, 436 (1972).
 (7) Gabelnick, Reedy, Chasanov, CPL 19, 90 (1973); JCP 58, 4468 (1973); 60, 1167 (1974).
 (8) Rauh, Ackermann, JCP 60, 1396 (1974).

US: ^aThermochemical value (mass-spectrom.)(1).
 (1) Cater, Rauh, Thorn, JCP 44, 3106 (1966); 48, 538 (1968)(Erratum).

V₂: ^aThermochemical value (mass-spectrom.)(1).
 (1) Kant, Lin, JCP 51, 1644 (1969).

V¹H, V²H:
 (1) Smith, PRS A 332, 113 (1973).
 (2) Scott, Richards, JP B 7, L347 (1974).
 (3) Henderson, Das, Wahl, JCP 63, 2805 (1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$51\text{V}^{14}\text{N}$		$\mu = 10.9839053_0$		$D_0^0 = 4.9_1 \text{ eV}^a$						JUN 1975
$51\text{V}^{16}\text{O}$		$\mu = 12.1729611_9$		$D_0^0 = 6.4_1 \text{ eV}^a$						JUN 1975
D	23980	[833]						$D \leftarrow X,^b$	23890	(18)
C $^4\Sigma^-$	17494.3	863.4 ^c (Z)	5.35	0.4953 ^{de}	0.0035	6	1.672 ₁	$C^f \leftrightarrow X,^{gh}$	R 17420.2	Z (1)(3)* (6)* (11)(12)(15) (17)*
B $^4\Pi(r)$	12760.8 12689 12625 12567	910.9	5.0	0.5246	0.004		1.625	$B \leftrightarrow X,^h$	R 12710.6 ⁱ 12638.6 12574.7 12516.7	H ^Q (2)(6)* (12) (15)(17)*
X $^4\Sigma^- k$	0	R shaded bands in the region 9470 - 9560 cm^{-1} . ^j						ESR sp. ^m		(4) (10)
		1011.3 ^c (Z)	4.86	0.54825 ^l	0.00352	6	1.5893 ₂			
$51\text{V}^{(32)}\text{S}$		$(\mu = 19.6437769)$		$D_0^0 = 4.6_2 \text{ eV}^a$						JUN 1975
$51\text{V}^{(80)}\text{Se}$		$(\mu = 31.111488_5)$		$D_0^0 = 3.5_4 \text{ eV}^a$						JUN 1975
$(184)\text{W}^{16}\text{O}$		$(\mu = 14.7153823_1)$		$D_0^0 = 6.8 \text{ eV}^a$						JUL 1975
		R shaded bands in gas phase emission from 12900 to 24400 cm^{-1} .								(1)(2)(3)(5)
G		[933]						$G \leftarrow X,$	23794	(6)
F		[982] ^b	c					$F \leftarrow X,$	23366	(6)
E		[944] ^b	c					$E \leftarrow X,$	21509	(6)
D	20834.2	993.0	H	6.5				$D \leftrightarrow X,$	R 20799.9	H (1)(6)
C		[931]	c					$C \leftarrow X,$	19190	(6)
B		[955] ^d	c					$B \leftarrow X,$	17283	(6)
A		[951] ^e	c					$A \leftarrow X,$	17132 ^e	(6)
X	0	1059.9	H	3.1						

Observed in absorption in rare gas matrices (6). Frequencies are for solid neon, except for $D \rightarrow X$ which was also identified (1) in the gas phase spectrum.

VN: ^aThermochemical value (mass-spectrom.)(1).
 (1) Farber, Srivastava, JCS FT I 69, 390 (1973).

VO: ^aThermochemical value (mass-spectrom.)(5)(9)(14)(19).
^bLow temp. matrix abs.; not observed in the gas phase.
^cFrom (17). Slightly different constants in (15).
^dSpin splitting constants (7)(15) for $v=0$: $\lambda = +0.53$,
^ePerturbations. $\gamma_1 = -0.009$, $\gamma_2 = -0.007$.
^fRadiative lifetime $\tau(v=0,1) = 0.41 \mu s$ (16).
^gAbsolute transition moments, band oscillator strengths
 (17). This ref. contains a useful review and bibliography of earlier work.
^hThe existence of a new system between 13900 and 14500 cm^{-1} , tentatively identified by Grosjean and Rosen [see (6)], is doubtful since the 2-0 and 0-3 sequences of B-X and C-X, respectively, are expected to overlap in this region.
ⁱSubband origin at 12706.8 cm^{-1} .
^jIt is not certain whether these bands form a new system or are part of B-X.
^kThe ESR spectrum of matrix isolated VO (10) is compatible only with a $^4\Sigma^-$ ground state, confirming theoretical predictions by (8).
^lSpin splitting constants (7)(15) for $v=0$: $\lambda = +1.371$, $\gamma_1 = +0.0112$, $\gamma_2 = +0.0111$. Large nuclear magnetic hfs, $b = 0.080 \text{ cm}^{-1}$ (10)(13). An unusual perturbation occurs in $v=0,1$ between F_2 and F_3 levels with $\Delta N = \Delta F = 0$ (13).
^mIn argon matrix.
 (1) Mahanti, PPS 47, 433 (1935).
 (2) Keenan, Schroeder, ApJ 115, 82 (1952).
 (3) Lagerqvist, Selin, Naturw. 42, 65 (1955); AF 12, 553
 (4) Lagerqvist, Selin, AF 11, 429 (1956). (1957).
 (5) Berkowitz, Chupka, Inghram, JCP 27, 87 (1957).
 (6) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

VO (continued):

- (7) Hougen, CJP 40, 598 (1962).
- (8) Carlson, Moser, JCP 44, 3259 (1966).
- (9) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).
- (10) Kasai, JCP 49, 4979 (1968).
- (11) Laud, Kalsulkar, IJP 42, 61 (1968).
- (12) Richards, Barrow, Nature 217, 842 (1968).
- (13) Richards, Barrow, Nature 219, 1244 (1968).
- (14) Frantseva, Semenov, HT(USSR) 7, 52 (1969).
- (15) Richards, D. Phil. Thesis (Oxford, 1969); see DONNSPEC.
- (16) Diebold, Wentink, unpubl.(1970); quoted in (17).
- (17) Harrington, Seel, Hebert, Nicholls, IAMS 7 (1970).
- (18) Weltner, unpubl.; quoted by Barrow in DONNSPEC.
- (19) Farber, Uy, Srivastava, JCP 56, 5312 (1972).
- (20) Veseth, PS 12, 125 (1975).

VS: ^aThermochemical value (mass-spectrom.)(1). Slightly higher value in (2).

- (1) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).
- (2) Owzarski, Franzen, JCP 60, 1113 (1974).

VSe: ^aThermochemical value (mass-spectrom.)(1); no details.
 (1) Bergman, Coppens, Drowart, Smoes, TFS 66, 800 (1970).

WO: ^aThermochemical value (mass-spectrom.)(4).

- ^bStrong interaction between levels of E and F.
- ^cHigher ΔG and deperturbed values may be found in (6).
- ^dStrong interaction between levels of A and B.
- ^eLowest observed level ($v=3?$) and ΔG . Weak system; the intensities of the bands derive mostly from the strong A \sim B interaction.

References on p. 661.

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4} cm^{-1})	r_e (\AA)	Observed Transitions		References		
								Design.	ν_{00}			
(129, 132) Xe_2										NOV 1977		
		$(u = 65.193611_g)$		$D_0^0 = 0.0230 \text{ eV}^a$		$\text{I.P.} = 11.12_7 \text{ eV}^b$						
		Several diffuse emission bands and continua in the visible and near UV regions; interpretation and assignment to Xe_2 uncertain.									(3)(5)	
K	85139.6	26	1	Associated with $7s[1\frac{1}{2}]_2^0$		(85189.31 cm^{-1}) c		$K \leftarrow X,^d$	85141.9	(19)		
		Unclassified abs. bands, associated with		{		$5d[1\frac{1}{2}]_1^0$ (83890.47 cm^{-1}) c $5d[2\frac{1}{2}]_3^0$ (82430.72 cm^{-1}) c		e		(19)(20)*		
H	82001	[30.0]		Associated with $5d[2\frac{1}{2}]_2^0$		(81926.04 cm^{-1}) c		$H \leftarrow X,^f$	82005.7	(19)		
		Unclassified abs. bands, associated with		{		$5d[1\frac{1}{2}]_2^0$ (80323.28 cm^{-1}) c $6p[0\frac{1}{2}]_0$ (80119.47 cm^{-1}) c $5d[0\frac{1}{2}]_1^0$ (79987.16 cm^{-1}) c		e		(9)(19)		
				{		$6p[1\frac{1}{2}]_2$ (79212.97 cm^{-1}) c $6p[1\frac{1}{2}]_1$ (78956.54 cm^{-1}) c $6p[2\frac{1}{2}]_3$ (78403.56 cm^{-1}) c $6p[2\frac{1}{2}]_2$ (78120.30 cm^{-1}) c		g		(20)*		
		Unclassified abs. bands, associated with		$6s'[0\frac{1}{2}]_1^0$		(77185.56 cm^{-1}) c		h		(14)		
B ($1\Sigma_u^+$) 0_u^+		Unclassified absorption bands longward and shortward of the resonance line at 68045.66 cm^{-1} (1469.6 \AA); pressure broadening of this line due to molecule formation. Continuous emission 68000 - 50000 cm^{-1} (1470 - 2000 \AA) with maxima near 68030, 67070 cm^{-1} (1470, 1491 \AA , "first continuum") and $\sim 58800 \text{ cm}^{-1}$ (1700 \AA , "second cont.")									$B^i \leftrightarrow X,^j$	(1)(2)(3)*
A ($3\Sigma_u^+$) 1_u												
X $1\Sigma_g^+$	0	21.12	H 0.65 ^d				4.36 ₁ ^m					

Xe₂: ^aSpectroscopic value, by extrapolation from the observed lowest ten vibrational levels of the ground state (20). The corresponding well depth is in very good agreement with $D_e^0 = 0.0243 \text{ eV}$ derived by (18) from bulk properties

and differential scattering cross sections as well as spectroscopic data. Integral absorption measurements of the 1274.8 \AA band (78444 cm^{-1}) as a function of temperature give $D_0^0 = 0.029 \text{ eV}$ (25).

Xe₂ (continued):

- ^bPhotoionization of Xe₂ (28). An earlier determination based on the formation of Xe₂⁺ from Rydberg excited Xe (associative ionization) yielded 11.14 eV (7).
- ^cAtomic energy levels relative to 5p⁶1S.
- ^dSeveral v" progressions (presumably v'=0...4) near 1174 Å.
- ^eBands longward of 1192 and 1250 Å have been partially analyzed by (19)(20); the ground state vibrational levels of (20) are from this analysis.
- ^fTwo v" progressions shortward, and two broad bands longward, of 1221 Å.
- ^g(25) have determined the oscillator strength (f = 0.03_g) for a band at 1274.8 Å.
- ^hContinuous absorption and ill defined vibrational structure longward of 1296 Å; small number of sharp bands at shorter wavelengths.
- ⁱRadiative lifetimes: A 100 ns [theoretical value of 23 ns predicted by (17)], B 6 ns (21)(26)(27). A and B are associated with the lowest excited states of Xe I, i.e. 6s[1½]₂^o (67068.05 cm⁻¹) and 6s[1½]₁^o (68045.66 cm⁻¹), respectively.
- ^jThe continuum is observed in discharges at high pressure as well as in fluorescence excited by the Xe I 1470 Å resonance line (12), by CO fourth positive bands (23), and by synchrotron radiation (24). There is good evidence that the "first continuum" is due to vibrationally unrelaxed molecules in the A and B states, while the "second continuum" corresponds to transitions from v'≈0

of these states to the steep repulsive part of the X 1Σ_g⁺ potential curve (11)(22). A broad emission peak at 1725 Å, probably representing the same transition, has been observed by bombardment of Xe in a Ne matrix with α particles (22) estimates r_e ≈ 3.25 Å. (16).

^lw_ey_e = +0.003. Zero point energy 10.40 cm⁻¹; last stable vibrational level (extrapol.) v=25 (20).

^mFrom bulk properties and differential scattering cross sections (18) [see (20), "note added in proof"]; see also (15). Electron diffraction (10) gives 4.41 Å.

- (1) McLennan, Turnbull, PRS A 132, 683 (1933).
- (2) Tanaka, Zelikoff, JOSA 44, 254 (1954).
- (3) Wilkinson, Tanaka, JOSA 45, 344 (1955).
- (4) Tanaka, JOSA 45, 710 (1955).
- (5) Roth, Gloersen, JCP 29, 820 (1958).
- (6) Huffman, Larrabee, Tanaka, AO 4, 1581 (1965).
- (7) Samson, Cairns, JOSA 56, 1140 (1966).
- (8) Wilkinson, JQSRT 6, 823 (1966).
- (9) Herzberg, unpublished.
- (10) Audit, JP(Paris) 30, 192 (1969).
- (11) Mulliken, JCP 52, 5170 (1970).
- (12) Freeman, McEwan, Claridge, Phillips, CPL 10, 530 (1971).
- (13) Kosinskaya, Polozova, OS(Engl. Transl.) 30, 458 (1971).
- (14) Castex, Damany, CPL 13, 158 (1972); 24, 437 (1974).
- (15) Docken, Schafer, JMS 46, 454 (1973).

(continued p. 662)

- WO (continued):
- (1) Gatterer, Krishnamurty, Nature 169, 543 (1952).
 - (2) Vittalachar, Krishnamurty, CS 23, 357 (1954).
 - (3) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

- (4) DeMaria, Burns, Drowart, Inghram, JCP 32, 1373 (1960).
- (5) Foster, Gaydon, quoted in IDSPEC (1963).
- (6) Weltner, McLeod, JMS 17, 276 (1965).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(129,132)Xe₂⁺										
		$(\mu = 65.193474_6) \quad D_0^0 = 1.02_6 \text{ eV}^a$							NOV 1977 A	
		Diffuse emission bands 61690 - 63130 cm^{-1} in a condensed discharge through Xe, tentatively assigned to Xe ₂ ⁺ .							(1)*	
D (² Σ _g ⁺) ¹ / ₂ g	(17500)	$D_0 \approx 0.17 \text{ eV}$		Preliminary data from the photoelectron spectrum (6). For an evaluation of difference potentials from g-u oscillations in the differential elastic scattering cross section see (4)(4b). Absolute photodissociation cross sections 14400 - 17700 cm^{-1} (5).				B ← X	(5)	
C (² Π _u) ¹ / ₂ u	(16700)	$D_0 \approx 0.26 \text{ eV}$								
	(8600)	Repulsive.								
B (² Π _g) ³ / ₂ g	(7000)	$D_0 \approx 0.16 \text{ eV}$								
	(5300)	$D_0 \approx 0.37 \text{ eV}$								
X (² Σ _u ⁺)	0							(3.25) ^b		
(132)Xe(⁷⁹)Br										
		$(\mu = 49.376402_4)$							NOV 1977	
B (² Σ ⁺)	36010 ^a	120	(0.23)				(2.96)	B ↔ X, ^b	(1)(2)(6)	
		Broad unclassified emission bands at 21500 and 28300 cm^{-1} . ^c							(1)(2)	
X (² Σ ⁺)	0	Repulsive state with van der Waals minimum of unknown depth.								
(132)Xe³⁵Cl										
		$(\mu = 27.6410016) \quad D_0^0 = 0.030_0 \text{ eV}^a$							NOV 1977	
D (¹ / ₂)								D ↔ X, ^b 42450	(8)	
B (² Σ ⁺)	32405.0	195.2	H 0.54				(2.94) ^c	B ↔ X, ^d v 32489.3 H	(2)(3)(4)(5)	
X (² Σ ⁺)	0	26.3	H -0.28 ^e				(3.18) ^c	ESR sp. ^f	(7)	

Xe $_2$ (continued):

- (16) Gedanken, Raz, Jortner, JCP 52, 1630 (1973).
- (17) Weihofen, JCP 60, 445 (1974).
- (18) Barker, Watts, Lee, Schafer, Lee, JCP 61, 3081 (1974).
- (19) Castex, CP 5, 448 (1974).
- (20) Freeman, Yoshino, Tanaka, JCP 61, 4880 (1974).
- (21) Keto, Gleason, Walters, PRL 33, 1365 (1974).
- (22) Mulliken, RR 59, 357 (1974).

Xe $_2$ (continued):

- (23) Fink, Comes, CPL 30, 267 (1975).
- (24) Brodmann, Zimmerer, Hahn, CPL 41, 160 (1976); Brodmann, Zimmerer, JP B 10, 3395 (1977).
- (25) Chashchina, Shreider, ZPS 25, 163 (1976). | (1976).
- (26) Keto, Gleason, Bonifield, Walters, Soley, CPL 42, 125
- (27) Leichner, Palmer, Cook, Thieneman, PR A 13, 1787
- (28) Ng, Trevor, Mahan, Lee, JCP 65, 4327 (1976) | (1976).

Xe_2^+ : ${}^aD_0^0(\text{Xe}_2) + \text{I.P.}(\text{Xe}) - \text{I.P.}(\text{Xe}_2)$. Values of 0.97 and 0.99 eV for D_e^0 have been derived by (3) and (4) from elastic scattering of Xe^+ by Xe using ground state r_e values which differ slightly from the one given in the Table.

b Estimated value (4a).

- (1) Tanaka, JOSA 45, 710 (1955).
- (2) Mulliken, JCP 52, 5170 (1970).
- (3) Lorents, Olson, Conklin, CPL 20, 589 (1973).
- (4) Mittmann, Weise, ZN 29 a, 400 (1974).
- (4a) See ref. (22) of Xe_2 .
- (4b) Jones, Conklin, Lorents, Olson, PR A 10, 102 (1974).
- (5) Miller, Ling, Saxon, Moseley, PR A 13, 2171 (1976).
- (6) Dehmer, Dehmer, JCP 67, 1774 (1977).

XeBr : a Energy of the potential minimum relative to $\text{Xe}({}^1S) + \text{Br}({}^2P_{3/2})$. All constants derived (6) by trial-and-error matching of observed and theoretically simulated spectra.

b Structured continuum with principal peak at 35480 cm^{-1} , observed in emission in the reaction of metastable (3P_2) Xe atoms with Br_2 , CH_2Br_2 , and PBr_3 at ~ 1 torr (1)(3) or on electron bombardment of Ar-Xe- Br_2 or Xe-HBr mixtures at pressures of the order of 1 atm (2)(6). Under the latter conditions laser action has been found (4)(6). Observed in absorption in an Ar matrix at 34000 cm^{-1} (5).

c (5) report emission peaks in argon matrices at 21200 and 26700 cm^{-1} .

- (1) Velazco, Setser, JCP 62, 1990 (1975).
- (2) Brau, Ewing, JCP 63, 4640 (1975).
- (3) Golde, JMS 58, 261 (1975).
- (4) Searles, Hart, APL 27, 243 (1975); 28, 602 (1976).

XeBr (continued):

- (5) Ault, Andrews, JCP 65, 4192 (1976).
- (6) Tellinghuisen, Hays, Hoffman, Tisone, JCP 65, 4473 (1976).

XeCl : a Extrapolation of the vibrational levels in $X \Sigma$ (5).

b Observed in a low-pressure discharge through $\text{Xe} + \text{Cl}_2$ (8). Absorption bands at similar wavelengths are observed in inert gas matrices (6).

c Based on potential functions chosen for best representation of observed levels and intensities (5).

d Observed in emission in the reaction of metastable (3P_2) Xe atoms with Cl_2 , NOCl , SOCl_2 , CCl_4 (2)(3) or on electron bombardment of mixtures of Ar+Xe+ Cl_2 and Xe+HCl or Cl_2 at high pressure (of the order of 1 atm) (4)(5). Under the latter conditions laser action has been detected (1)(5). Observed in absorption and emission in inert gas matrices (6).

${}^e\omega_e y_e = -0.067$.

f In argon at 4.2 K.

- (1) Ewing, Brau, APL 27, 350 (1975).
- (2) See ref. (3) of XeBr .
- (3) See ref. (1) of XeBr .
- (4) See ref. (2) of XeBr .
- (5) Tellinghuisen, Hoffman, Tisone, Hays, JCP 64, 2484 (1976).
- (6) See ref. (5) of XeBr .
- (7) Adrian, Bowers, JCP 65, 4316 (1976).
- (8) Shuker, APL 29, 785 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-4} cm $^{-1}$)	r_e (Å)	Observed Transitions		References
								Design.	v_{00}	
(132)Xe19F										
		$(\mu = 16.6065342)$		$D_0^0 = 0.13_3$ eV ^a		$I.P. \leq 10.23$ eV ^b				NOV 1977 A
D ($^2\Pi_{1/2}$)	38057	351	H 2.1					D \leftrightarrow X, ^c V	38118 H	(2)(7)(13) (16)*
B ($^2\Pi_{1/2}$)	28826	308.6	(Z) 1.52					B ^d \leftrightarrow X, ^e V	28866	(2)(5)* (7) (9)(12)(13)
C ($^2\Pi_{3/2}$)	(25550)	(370)	} Tentative interpretation (10) of observations in solid argon.					{ C \rightarrow A, (18600) C \leftarrow X, (25620)		(10)
A ($^2\Pi_{3/2}$)		Unstable								
X ($^2\Sigma$)	0	234.2 ^f	(Z) 12.0					ESR sp. ^g		(1)(3)
(132)Xe19F$^+$										
		$D_0^0 \geq 2.03$ eV ^a								NOV 1977
(132)Xe1H										
		$(\mu = 1.00018323)$		$D_e^0 = 0.0068_3$ eV ^a						NOV 1977
X $^2\Sigma$	0	Evidence for the existence of quasibound levels in the van der Waals well [orbiting resonances in the in- tegral scattering cross section (3)].					3.9 ₄ ^a			
(132)Xe1H$^+$										
		$D_e^0 = (4.32)$ eV ^a								NOV 1977
X $^1\Sigma$	0							(1.59) ^a		

XeF: ^aFrom (12) after correction for change in the v numbering of the ground state. Extensive ab initio calculations (4) suggested an essentially repulsive pot. for X $^2\Sigma$; much better agreement with the spectroscopic result is obtained (11) if, in addition, the contribution to binding from the dispersion interaction is taken into $D_0^0(\text{XeF}) + \text{I.P.}(\text{Xe}) - D_0^0(\text{XeF}^+)$. | account.
^cObserved in emission in the reaction of metastable rare gas atoms with fluorine containing molecules (13)(16) and in electron-beam excited mixtures of Ar+Xe+F₂ at

XeF (continued):

high total pressure (7). Absorption in inert gas matrices at similar wavelengths (10). Laser-excited emission spectra in solid Ne and Ar (14); lifetimes of 12.5 and 11.5 ns, respectively, have been measured.

^dLifetime $\tau = 18.8$ ns (15); (14) measure 6 ns in solid Ar.

^eObserved in emission at low pressure in the reaction of metastable (3P_2) Xe atoms with F₂, NOF, N₂F₄, CF₃OF [flowing afterglow (6)(9)] and at high pressure (of the order

XeF (continued):

of 1 atm) on electron bombardment of mixtures of Ar, Xe, and F₂ or NF₃ (5)(7)(12); two bands (0-3 and 1-4 according to the new v" numbering) at 3532 and 3511 Å show strong laser action (5)(8)(12). Also observed in fluorescence in the photolysis of XeF₂ (17). In emission and absorption in inert gas matrices (10)(14).

^fThe v" numbering in (12) has been changed in a "note added in proof". See also (16). Emission spectra in a neon matrix (14) give $\omega_e = 247$, $\omega_e x_e = 10.2$.

^gIn γ -irradiated solid XeF₄ and XeF₂ (1)(3).

- (1) Morton, Falconer, JCP 39, 427 (1963).
- (2) Kuznetsova, Kuzyakov, Shpanskii, Khutoretskii, VMUK 19, 19 (1964).
- (3) Eachus, Symons, JCS A (1971), p. 304.
- (4) Liskow, Schaefer, Bagus, Liu, JACS 95, 4056 (1973).
- (5) Ault, Bradford, Bhaumik, APL 27, 413 (1975).
- (6) Velazco, Setser, JCP 62, 1990 (1975).
- (7) Brau, Ewing, JCP 63, 4640 (1975).
- (8) Brau, Ewing, APL 27, 435 (1975).
- (9) Golde, JMS 58, 261 (1975).
- (10) Ault, Andrews, JCP 64, 3075 (1976); 65, 4192 (1976).
- (11) Krauss, Liu, CPL 44, 257 (1976).
- (12) Tellinghuisen, Tisone, Hoffman, Hays, JCP 64, 4796 (1976).
- (13) Velazco, Kolts, Setser, JCP 65, 3468 (1976).
- (14) Goodman, Brus, JCP 65, 3808 (1976).
- (15) Burnham, Harris, JCP 66, 2742 (1977).
- (16) Velazco, Kolts, Setser, Coxon, CPL 46, 99 (1977).
- (17) Brashears, Setser, Desmarteau, CPL 48, 84 (1977).

XeF⁺: ^aFrom photoionization data (3). XeF⁺ is formed in the photoionization of XeF₂ (1)(3) and in the reaction $\text{Xe}^+(^2P_{3/2,1/2}) + \text{F}_2 = \text{XeF}^+ + \text{F}$ (2).

- (1) Morrison, Nicholson, O'Donnell, JCP 49, 959 (1968).
- (2) Berkowitz, Chupka, CPL 7, 447 (1970).
- (3) Berkowitz, Chupka, Guyon, Holloway, Spohr, JPC 75, 1461 (1971).

Xe¹H: ^aScattering of H atoms by Xe (2). The repulsive potential at higher energies has been determined by (1).

- (1) Picot, Fink, JCP 56, 4241 (1972).
- (2) Bickes, Lantzsich, Toennies, Walaschewski, FDCS No. 55, 167 (1973).
- (3) Toennies, Welz, Wolf, JCP 61, 2461 (1974).

Xe¹H⁺: ^aFrom the ab initio calculations of (2); D_e⁰ refers to Xe⁺ + H and has been reduced by 1.47 eV from the value given in (2) [Xe + H⁺]. See also (3). The proton scattering results of (1) are energy dependent, probably because of charge exchange in the curve crossing region.

- (1) Weise, Mittmann, Ding, Henglein, ZN 26 a, 1122 (1971).
- (2) Kubach, Sidis, JP B 6, L289 (1973).
- (3) Gallup, Macek, JP B 10, 1601 (1977).

State	T_e	w_e	$w_{e^+e^-}$	B_e	α_e	D_e (10^{-1} cm^{-1})	r_e (\AA)	Observed Transitions		References	
								Design.	v_{00}		
(132)Xe¹²⁷I											
B ($^2\Sigma^+$)	40210 ^a	112	(0.24)	Diffuse emission bands with principal peak at 39510 cm^{-1} . Broad diffuse bands at 27770 and 30760 cm^{-1} . Unstable.			(3.31)	B \rightarrow X, ^b B \rightarrow A, ^b	NOV 1977 (2)(3)(4) (2)(3)		
A ($^2\Pi_{3/2,1/2}$)											
X ($^2\Sigma^+$)	0	Repulsive state with van der Waals minimum of unknown depth.									
(132)Xe¹⁴N ?											
		($\mu = 12.6591650_4$)	Emission system at 20300 cm^{-1} , observed in a d.c. discharge through Xe + N ₂ .						NOV 1977 (1)		
(132)Xe¹⁶O											
F		($\mu = 14.2651049_3$)	Broad emission continuum with maximum at 42200 cm^{-1} , in discharges through Xe + trace of O ₂ and in chemiluminescence of Xe(³ P ₂) + N ₂ O. Narrow band group at 34300 cm^{-1} in discharges through Xe + O ₂ . Laser excitation produces a broad emission band at 34500 cm^{-1} in solid argon.					F \leftrightarrow X, ^a (F \rightarrow A)	NOV 1977 (1b)(4)(5) (2)(13)		
d ($^1\Sigma^+$)	(33268) ^b	152	H	9.9	<u>Ab initio</u> potential functions (12). The molecular states arise from Xe(¹ S) + O(¹ S): d, Xe(¹ S) + O(¹ D): a, b, c, Xe(¹ S) + O(³ P): X, A.			d \rightarrow b, ^c (17695) ^d d ^e \rightarrow a, ^f R 20097 ^g H	(8)(13) (1)(1a)(1b) (3)* (13)		
c ($^1\Delta$)								(d \rightarrow X) ^h 32460	(1b)(8)(13)		
b ($^1\Pi$)	(15600) ^b	97 ^d	H	8.7							
a ($^1\Sigma^+$)	(13068) ^b	372 ^g	H	12.0							
A ($^3\Sigma^-$)		Repulsive state.									
X ($^3\Pi$)		Repulsive state.									

XeI: ^aEnergy of the potential minimum relative to Xe(¹S) + I(²P_{3/2}). All constants obtained by trial-and-error matching of observed and calculated spectra (4).
^bObserved in the reaction of metastable Xe (³P₂) atoms with I₂ and CF₃I (1) and when Xe+HI or Ar+Xe+I₂ mixtures at high pressure (~1 atm) are bombarded by electrons (2)(4).
 (1) Velazco, Setser, JCP 62, 1990 (1975).
 (2) Brau, Ewing, JCP 63, 4640 (1975).
 (3) Ewing, Brau, PR A 12, 129 (1975).
 (4) Tellinghuisen, Hays, Hoffman, Tisone, JCP 65, 4473 (1976).
 XeN: (1) Herman, Herman, Nature 193, 156 (1962).
 XeO: ^aCharge-transfer transition from a largely ionic upper state (⁺XeO⁻) to the largely atomic ground state; see (5). In argon matrix absorption at 44040 cm⁻¹ (10).
^bT_e relative to Xe(¹S) + O(³P₂).
^cObserved in emission from electron-beam excited high-density Xe + O₂ mixtures (8) and as laser-excited fluorescence in rare gas matrices (13).
^dThe b state vibrational numbering (8) is uncertain; according to (13) it may have to be increased by +1.
^eLifetime τ(v=0,1) ≈ 50 μs (7); (9) suggest the much shorter value τ ≈ 0.1 μs.
^fObserved in an ozonizer-type discharge through Xe (~1 atm) + traces of O₂ (3); partially resolved rotational structure. Laser-excited fluorescence in rare gas matrices (13). Laser oscillation observed using electron-beam excitation of high-pressure Xe containing small amounts of O₂ (6)(11).

XeO (continued):

^gThe a state vibrational numbering (3) may have to be raised by +3 units; an unambiguous numbering has not been established in spite of the availability of Xe¹⁸O data in solid argon (13).
^hNarrow emission peak; in solid argon and neon at 31940 and 32670 cm⁻¹, respectively.
 (1) Kenty, Aicher, Noel, Poritsky, Paolino, PR 69, 36 (1946).
 (1a) Herman, CR 222, 492 (1946).
 (1b) Herman, Herman, JPR 11, 69 (1950).
 (2) Cuthbertson, Herman, CR 234, 1355 (1952).
 (3) Cooper, Cobb, Tolnas, JMS 7, 223 (1961).
 (4) Stedman, Setser, JCP 52, 3957 (1970).
 (5) Golde, Thrush, CPL 29, 486 (1974).
 (6) Powell, Murray, Rhodes, APL 25, 730 (1974).
 (7) Tisone, JCP 60, 3716 (1974).
 (8) Lorents, Huestis, in Lecture Notes in Physics, Vol. 43; Laser Spectroscopy, p.100 (Springer, Berlin 1975).
 (9) Aleksandrov, Vinogradov, Lugovskii, Podmoshenskii, OS(Engl. Transl.) 41, 224 (1976).
 (10) Ault, Andrews, CPL 43, 350 (1976).
 (11) Basov, Babeiko, Zuev, Mikheev, Orlov, Pogorelskii, Stavrovskii, Startsev, Yalovoi, SJQE 6, 505 (1976).
 (12) Dunning, Hay, JCP 66, 3767 (1977).
 (13) Goodman, Tully, Bondybey, Brus, JCP 66, 4802 (1977).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	v_{00}	
$^{89}\text{Y}_2$		$\mu = 44.452933_4$ $D_0^0 = 1.6_2 \text{ eV}^a$							JUL 1975	
$(^{172},^{174})\text{Yb}_2$		$(\mu = 86.465923)$ $D_0^0 = 0.1_7 \text{ eV}^a$							JUL 1975	
$(^{174})\text{Yb}(^{35})\text{Cl}$		$(\mu = 29.1154527)$							JUL 1975 A	
B ($^2\Sigma$) ^a 19928.0		315.0	H	2.0	(fragment only)			B \rightarrow X, V 19939.1 H	(1)	
$A_2(^2\Pi)$ ^a { 19369.3		314.6	H	1.38				$A_2\rightarrow$ X, V 19380.0 H	(1)*	
A_1 { 17882.0 ^b		314.4	H	1.12 ^c				$A_1\rightarrow$ X, V 17892.1 H	(1)*	
X ($^2\Sigma$) ^a 0		293.6 ^d	H	1.23 ^d						
$(^{174})\text{Yb}^{19}\text{F}$		$(\mu = 17.1276445)$ $D_0^0 = 4.8 \text{ eV}^a$							SEP 1976 A	
B ($^2\Sigma^+$) $\frac{1}{2}$ (21067)		[511.75]	H	b	[0.2486] ^c		[1.990]	B \leftrightarrow X, V 21074.25 ^d H	(2)	
$A_2(^2\Pi)$ { $\frac{3}{2}$ (19460)		[540.35]	H	b	[0.24863]	[3.16] ^e	[1.9896]	$A_2\leftrightarrow$ X, V 19470.99 ^f Z	(2)*	
A_1 { $\frac{1}{2}$ (18090)		[473.72]	H	b	[0.2470 ₄] ^g	[2.1 ₄]	[1.996 ₀]	$A_1\leftrightarrow$ X, V 18106.28 ^f Z	(2)	
X $^2\Sigma^+$ 0		[501.91]	Z	2.20 ₅	[0.24140]	0.0015	[2.18] 2.0161			

Y₂: ^aThermochemical value (mass-spectrom.)(1).
 (1) Verhaegen, Smoes, Drowart, JCP 40, 239 (1964).

Yb₂: ^aThermochemical value (mass-spectrom.)(1).
 (1) Guido, Balducci, JCP 57, 5611 (1972).

YbCl: ^aAssignments by analogy with YbF (2).
^b(1) give 17800.9 which does not fit their data.
^c $\omega_e y_e = +0.0072$.
^dAverage of the constants from A₁-X and A₂-X.
 (1) Gatterer, Piccardi, Vincenzi, RS 1, 181 (1942).
 (2) See ref. (2) of YbF.

YbF: ^aCorrected (1) linear Birge-Sponer extrapolation for the ground state (2). See, however, (3) who derive $D_0^0 \geq 5.36$ eV from the Yb + F₂ chemiluminescence spectrum.
^bHigher ΔG values in (2); strong perturbations.
^cLarge perturbations.
^dHead nearest to origin.
^e $H_0 = +4.1 \times 10^{-12}$.
^f{J'=0} relative to N''=0.
^gΩ-type doubling $\Delta v_{fe} = -0.40(J+\frac{1}{2})$.
 (1) Hildenbrand, AdHTC 1, 193 (1967).
 (2) Barrow, Chojnicki, JCS FT II 71, 728 (1975).
 (3) Yokozeiki, Menzinger, CP 14, 427 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-5}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
(174)Yb ¹ H										
		($\mu = 1.00201939$)		$D_0^0 \approx (1.93) \text{ eV}^a$						JAN 1976 A
F $\frac{1}{2}^b$				$[4.155]^c$		$[16.6]$	$[2.012]$	$F \leftrightarrow X, \text{ v}$	22002.39^d Z	(2)(6)
E ($2\Sigma^+$) $\frac{1}{2}$				$[4.2497]^e$		$[19.7]$	$[1.9897]$	$E \leftrightarrow X, \text{ v}$	17822.56^d Z	(2)* (3)(6)
D (2Π) $\left\{ \begin{array}{l} \frac{3}{2} \\ \frac{1}{2} \end{array} \right.$	16780	$[1319.7]$	Z (19.4)	4.1609^f	0.088_6	$[14.68]^g$	2.0108	D $\leftrightarrow X, \text{ v}$	16834.72^d Z	(1)(2)
	15325.6	$[1307.5_4]$	Z 21.0_2^h	4.1950^i	0.089_8^h	$[15.33]^j$	2.0026		15375.58^d Z	(1)(2)* (3)(6)
C ($\Omega > \frac{1}{2}$) ≤ 15200		$\geq 1500^k$	(30)	$(4.4)^k$						(2)
B ($\frac{1}{2}$) ≤ 15400		$\geq 1370^l$		$(3.2)^l$						(2)(4)
a $\left\{ \begin{array}{l} 4\Sigma_{3/2}^+ \\ 4\Sigma_{1/2}^+ \end{array} \right.$		Not observed.		$[4.672_3]^m$		$[7.1]^n$	$[1.8976]$	a $\rightarrow X,$	13183.92^d Z	(5)(7)
X $2\Sigma^+$	0	1249.54	Z 21.06	3.9930_5^o	0.0956_5^p	16.18^q	2.0526			
(174)Yb ² H										
		($\mu = 1.99104715$)								JAN 1976 A
F $\frac{1}{2}^a$				$[2.1289]^b$		$[4.24]$	$[1.9943]$	$F \rightarrow X,^c \text{ v}$	21986.20^d Z	(2)* (3)(6)
E ($2\Sigma^+$) $\frac{1}{2}$	17768.6	968.65	Z 24.41	$[2.1425]^e$	f	$[-8]^g$	$[1.9879]$	$E \rightarrow X, \text{ v}$	17806.16^d Z	(2)(3)(6)
D (2Π) $\left\{ \begin{array}{l} \frac{3}{2} \\ \frac{1}{2} \end{array} \right.$	16778	$[945.50]$	Z (15.6)	$[2.09241]^h$	0.0472	$[3.962]^i$	2.0003	D $\rightarrow X, \text{ v}$	16822.18^d Z	(2)
	15326.4	957.9	Z 9.7	2.122^j	0.039	$[4.18]^k$	1.997		15362.3^d Z	(2)(7)
a $\left\{ \begin{array}{l} 4\Sigma_{3/2}^+ \\ 4\Sigma_{1/2}^+ \end{array} \right.$	13008.5	1084.4	Z 9.84	2.3516^l	0.0371	3.40^m	1.8975	a $\rightarrow X, \text{ v}$	13107.60^d Z	(5)(7)*
				$[2.1931]^n$		$[4.8]^o$	$[1.9648]$		12493.15^d Z	(3)(4)* (7)
X $2\Sigma^+$	0	886.6	Z 10.57	2.01162^p	0.03425^q	$[4.160]^r$	2.0516			

Yb¹H: ^aFrom the predissociation in D $\frac{1}{2}$ (v=0). The fact that a $^4\Sigma_{1/2}$ was not observed for Yb¹H may be due to predissociation; in this case D₀⁰ \approx 1.55 eV.
^bVeseth (6) suggests $\Omega = 3/2$.
^c Ω -type doubling, $\Delta v_{fe} = -0.23(J+\frac{1}{2}) + \dots$ (2). Different constants in (6). Perturbations.
^d{J'=0} relative to N''=0.
^eLarge Ω -type doubling, $\Delta v_{fe} = +13.60(J+\frac{1}{2}) - \dots$. f levels perturbed by v=2 of D $\frac{1}{2}$ (6).
^fPerturbations. Ω -type doubling, $\Delta v_{fe}(v=0) = +5.19 \times 10^{-4}(J-\frac{1}{2})(J+\frac{1}{2})(J+\frac{3}{2}) - \dots$.
^gD₁ = 16.5×10^{-5} ; H₁ = $+2.8 \times 10^{-8}$.
^hData for v=2 (B = 3.958) from a perturbation in the f levels of E, v=0. See (6).
ⁱ Ω -type doubling, $\Delta v_{fe}(v=0) = -4.89(J+\frac{1}{2}) + \dots$. Perturbations. An accidental predissociation occurs in v=0 near the intersection with a level of B ($\frac{1}{2}$).
^jD₁ = 15.7×10^{-5} .
^kFrom perturbations in the $\frac{1}{2}$ and $\frac{3}{2}$ components of D. Vibrational numbering unknown.
^lFrom perturbations in the e levels of D $\frac{1}{2}$, v=0 and 1. Vibrational numbering unknown.
^m Ω -type doubling, $\Delta v_{fe} = +0.0285_8(J-\frac{1}{2})(J+\frac{1}{2})(J+\frac{3}{2}) - \dots$.
ⁿAlso higher order constants.
^oSpin splitting $\Delta v_{12}(v=0) = +0.5688(N+\frac{1}{2}) - \dots$.
^p $\gamma_e = -0.0010_8$.
^q $\beta_e = +0.18 \times 10^{-5}$; H₀ = $+4.02 \times 10^{-9}$, H₁ = $+4.39 \times 10^{-9}$, H₂ = $+4.6 \times 10^{-9}$.
For ref. see Yb²H.

Yb²H: ^aSee ^b of Yb¹H.
^b Ω -type doubling, $\Delta v_{fe} = -0.231(J+\frac{1}{2}) + \dots$. Perturbations.
^cOne P, one R, and two Q branches.
^dSee ^d of Yb¹H.
^e Ω -type doubling, $\Delta v_{fe}(v=0) = +6.989(J+\frac{1}{2}) - \dots$ (2). Slightly different constants in (6). Perturbations.
^fB₁ = 2.104, B₂ = 2.013.
^gH₀ = -34×10^{-8} . Additional D_v, H_v values in (2).
^hPerturbations. Ω -type doubling, $\Delta v_{fe}(v=0) = +0.682 \times 10^{-4}(J-\frac{1}{2})(J+\frac{1}{2})(J+\frac{3}{2}) - \dots$; for v=1 see (2).
ⁱD₁ = 6.0×10^{-5} ; H₀ = $+5.0 \times 10^{-10}$, H₁ = $+4.9 \times 10^{-8}$.
^j Ω -type doubling, $\Delta v_{fe}(v=0) = -2.590(J+\frac{1}{2}) + \dots$. Perturbations by levels of $^4\Sigma_{3/2}^+$.
^kD₁, D₂ (10^{-5}cm^{-1}) = 3.80, 3.3₆; and higher order constants.
^l Ω -type doubling, $\Delta v_{fe}(v=0) = +0.00363_4(J-\frac{1}{2})(J+\frac{1}{2})(J+\frac{3}{2}) - \dots$.
^m $\beta_e \approx -0.09$; also higher order constants.
ⁿLarge Ω -type doubling, $\Delta v_{fe}(v=0) = -9.051(J+\frac{1}{2}) + \dots$.
^oAlso higher order constants.
^pSpin splitting $\Delta v_{12}(v=0) = +0.2876(N+\frac{1}{2}) - \dots$.
^q $\gamma_e = -0.000320$.
^rD₁ = 4.174×10^{-5} , H_e $\approx +6.3 \times 10^{-10}$.
(1) Kopp, Naturw. 49, 202 (1962).
(2) Hagland, Kopp, Åslund, AF 32, 321 (1966).
(3) Kopp, Hougen, CJP 45, 2581 (1967).
(4) Hagland, Kopp, AF 39, 257 (1969).
(5) L. Hagland, Thesis (Stockholm, 1969), quoted in DONNSPEC (1970).
(6) Veseth, JP B 6, 1484 (1973).
(7) Kopp, Hagland, Rydh, CJP 53, 2242 (1975); USIP Report 75 - 15 (July 1975).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$(174)\text{Yb}^{160}$		$(\mu = 14.6479335_3) \quad D_0^0 \leq 3.6_8 \text{ eV}^a \text{ or } \geq 4.08 \text{ eV}^b.$ Unclassified, mostly R shaded emission bands in the region $17700 - 21500 \text{ cm}^{-1}$.								SEP 1976 A (1)* (2)*
$^{89}\text{Y}^{35}\text{Cl}$		$\mu = 25.0974229$								JUL 1975
C $^1\Sigma$	14907.6	324.5	H 1.14	(0.1089) ^a	(0.0007)	(0.9) ^a	(2.48 ₄)	C \rightarrow X,	R 14879.5	H (1)
X $^1\Sigma^b$	0	380.7	H 1.3	(0.1160) ^a	(0.0003)	(0.9) ^a	(2.40 ₆)			
$^{89}\text{Y}^{19}\text{F}$		$\mu = 15.6534084 \quad D_0^0 = 6.2 \text{ eV}^a$								DEC 1976 A
G $^1\Pi$	31253.6	[536.30] (Z)	2.1 ₃	0.27661	0.00233	[2.96]	1.9731	G \leftrightarrow X,	R 31205.80	Z (1)(2)(3)(6)
F $^1\Sigma^+$	28022.5	552.9 H	2.6 ₉	[0.27536]		[2.76]	[1.9776]	F \leftrightarrow X,	R 27980.81	Z (2)(4)(7)
E $^1\Pi$	b	[581.92] (Z)		[0.27090] ^c	0.0024	[2.5]	[1.9938]	E \leftrightarrow X, (R)	25464.33	Z (3)(4)(6)
D $^1\Pi$	b			[0.26805] ^d		[3.3]	[2.0044]	D \leftrightarrow X,	R 25324.90	Z (3)(6)
C $^1\Sigma^+$	19242.4	[527.20] (Z)	2.45	0.26666	0.00177	[2.64]	2.0096	C \leftrightarrow X,	R 19190.35	Z (2)(3)(6)
b $^3\phi_4$ e	$a_2 + 15051.7$								15028.0	H
	$a_2 + 14865.9$	536.1 H	2.41	[0.277]			[1.97 ₂]	b \leftrightarrow a,	R 14842.8	H (2)(3)
	$a_1 + 14658.1$								14635.5	H
B $^1\Pi$	15934.2	[534.67] (Z)	2.35 ^f	0.26709 ^g	0.00156	[2.61]	2.0080	B \leftrightarrow X,	R 15885.78	Z (1)(2)(3)(4)(6)
a $^3\Delta_3$ e	a_3	583.5 H	2.49							
	a_2	582.3 H	2.42	[0.285]			[1.94 ₄]			
	a_1	581.2 H	2.39							
X $^1\Sigma^+$	0	[631.29] (Z)	2.50	0.29042	0.00163	[2.37]	1.9257			
$^{89}\text{Y}^{19}\text{F}^+$										DEC 1976
$^2\Pi(r)$	$x_2 + 28062.4$ $x_1 + 27964.0$	716.6 H [711.5 ₃] Z	2.38 2.41 H	[0.3065] [0.3055] ^h	0.0015	[2.0] [2.2]	[1.876 ₀]	$^2\Pi \rightarrow ^2\Delta$,	v 28088.37 Z 27990.3 ₄ Z	(7)
$^2\Delta(r)$	x_2 x_1	664.7 H 663.7 H	2.30 2.29	[0.2960] [0.2953]		[2.2] [2.2]	[1.908 ₆]			

YbO: ^aThermochemical value (mass-spectrom.)(3), recalc. (4).

^bFrom the Yb+O₃ chemiluminescence spectrum (5).

(1) See ref. (1) of YbCl.

(2) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).

(3) Ames, Walsh, White, JPC 71, 2707 (1967).

(4) Smoes, Coppens, Bergman, Drowart, TFS 65, 682 (1969).

(5) See ref. (3) of YbF.

YCl: ^aUncertain. The D values from the rotational analysis are approximately twice as large as the values calculated from $D = 4B^3/\omega^2$.

^bNot certain that this is the ground state.

(1) Janney, JOSA 56, 1706 (1966).

YF, YF⁺: ^aThermochemical value (mass-spectrom.)(5).

^bThe absorption spectrum in this region contains several overlapping bands, and it is not certain how many states are involved (3)(6). Perturbations.

^c Λ -type doubling (6), $\Delta v = 0.0007 \times J(J+1)$.

^d Λ -type doubling (6), $\Delta v = 0.00049 \times J(J+1)$.

^eAssignments by analogy with ScF.

^f1.61 in (2)(4).

^g Λ -type doubling (3)(6), $\Delta v_{ef} = (-)0.00013_2 \times J(J+1)$.

^h Λ -type doubling, $\Delta v = 0.0079(J+\frac{1}{2})$.

(1) Barrow, Gissane, PPS 84, 615 (1964).

(2) Shenyavskaya, Mal'tsev, Gurvich, OS(Engl. Transl.) 21, 374 (1966).

(3) Barrow, Bastin, Moore, Pott, Nature 215, 1072 (1967).

(4) Shenyavskaya, Mal'tsev, Gurvich, VMUK 22(4), 104 (1967).

(5) Zmbov, Margrave, JCP 47, 3122 (1967).

(6) R. F. Barrow, in DONNSPEC (1970).

(7) Shenyavskaya, Ryabov, JMS 63, 23 (1976).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{89}\text{Y}^{160}$										
		$\mu = 13.5560646_9$		$D_0^0 = 7.2_9 \text{ eV}^a$						JUL 1975 A
B $2\Sigma^+$	20791	765.5	H 8.0	[0.3722] ^b		[3.8]	[1.827 ₉]	B \leftrightarrow X, R	20741.9 ₂ Z	(1)(2)(3) (4)* (5)* (6)* (7)* (9)(11)(16) (17)(18)(19)
A $2\Pi_r$	16742.2 16315.0	822.7 ^c 820.7 ^c	3.9 ₇ 3.5 ₀	[0.3857] ^d	(0.0023)	[3.5]	[1.795 ₆]	A \leftrightarrow X, R	16722.7 ₅ ^e Z 16294.7 ₂ Z	(1)(2)* (3) (4)* (5)* (6)* (7)* (9)(11)(17) (18)
X $2\Sigma^+$	0	861.0 ^c	2.9 ₃	[0.3881] ^f	(0.0018)	[3.2]	[1.790 ₀]	ESR sp. ^g		
$^{89}\text{Y}^{(32)}\text{S}$										
		$(\mu = 23.5154972)$		$D_0^0 = 5.4_5 \text{ eV}^a$						JUL 1975
A 2Π	13971 13462	[438] [447]						A \leftarrow X, ^b	13949 13444	(2)
X 2Σ	0	[483]						b		
$^{89}\text{Y}^{(80)}\text{Se}$										
		$(\mu = 42.085933_4)$		$D_0^0 = 4.4_9 \text{ eV}^a$						JUL 1975
$^{89}\text{Y}^{(130)}\text{Te}$										
		$(\mu = 52.782392_8)$		$D_0^0 = 3.4_8 \text{ eV}^a$						JUL 1975

Y0: ^aThermochemical value (mass-spectrom.)(20), see also (8)
(10)(12)(13)(14)(15).

^bSpin-splitting constant $\gamma_0 = (-)0.148$.

^cRedetermined, taking into account estimated head-origin separations.

^d Λ -type doubling in $^2\Pi_{1/2}$, $\Delta v_{fe}(v=0) = -0.151(J+\frac{1}{2})$.

^e $\{J'=0\}$ relative to $N''=0$.

^fNuclear magnetic hyperfine structure; $b = -0.027 \text{ cm}^{-1}$
[from the ESR spectrum, (11)(18)].

^gIn rare gas matrices (11)(18).

- (1) Johnson, Johnson, PRS A 133, 207 (1931).
- (2) Meggers, Wheeler, JRNBS 6, 239 (1931).
- (3) Jevons, "Band Spectra of Diatomic Molecules", Phys. Soc. London (1932).
- (4) Piccardi, GCI 63, 127 (1933).
- (5) Gatterer, RS 1, 153 (1942).
- (6) See ref. (2) of Yb0.
- (7) Uhler, Åkerlind, AF 19, 1 (1961).
- (8) White, Walsh, Ames, Goldstein, in "Thermodynamics of Nuclear Materials", p. 417. IAEA, Vienna (1962).
- (9) Ortenberg, Glasko, SAAJ 6, 714 (1963);
Ortenberg, Glasko, Dimitriev, SAAJ 8, 258 (1964).
- (10) Ackermann, Rauh, Thorn, JCP 40, 883 (1964).
- (11) Kasai, Weltner, JCP 43, 2553 (1965).
- (12) Smoes, Drowart, Verhaegen, JCP 43, 732 (1965).
- (13) See ref. (3) of Yb0.
- (14) Coppens, Smoes, Drowart, TFS 63, 2140 (1967).
- (15) Drowart, Pattoret, Smoes, PBCS No. 8, 67 (1967).
- (16) Murthy, Murthy, PPS 90, 881 (1967).
- (17) Veits, Gurvich, DC 173, 377 (1967).
- (18) Weltner, McLeod, Kasai, JCP 46, 3172 (1967).
- (19) Dube, Rai, Singh, IJPAP 10, 87 (1972);
Dube, IJPAP 10, 167 (1972).
- (20) Ackermann, Rauh, JCP 60, 2266 (1974).

YS: ^aThermochemical value (mass-spectrom.)(1).

^bVisible, IR, and ESR spectra of YS in rare gas matrices at 4 K (2). Gas phase spectrum not observed.

(1) See ref. (14) of Y0.

(2) McIntyre, Lin, Weltner, JCP 56, 5576 (1972).

YSe: ^aThermochemical value (mass-spectrom.)(1).

(1) Ni, Wahlbeck, HTS 4, 326 (1972).

YTe: ^aThermochemical value, no details (1).

(1) Uy, Drowart, HTS 2, 293 (1970).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References	
								Design.	ν_{00}		
^(64,66) Zn ₂		$(\mu = 32.456117_9)$ Large number of continua and diffuse bands in emission and absorption. See (1).							JUL 1975 A		
⁽⁶⁴⁾ Zn ⁽⁷⁹⁾ Br		$(\mu = 35.318658_6)$							JUL 1975		
C (² Π)	32523 32125	358.0 ^a H 350.0 ^a H	2.00 2.00					C ↔ X, b	32543 ^a 32141 ^a	H H	(1)(2)(3)(5) (7)(8)
B (² Σ)		Unclassified bands from 11800 to 30000 cm ⁻¹ . ^c						B → X, R			(2)(4)(6)
X (² Σ)	0	318.0 ^a H	2.00								
⁽⁶⁴⁾ Zn ⁽³⁵⁾ Cl		$(\mu = 22.6043892)$ $D_0^0 = 2.1 \text{ eV}^a$							JUL 1975		
E (² Σ)	(48186.4)	(345.4)	(5.0)					E → X, ^b R	48163.0 (Z)		(4)
C (² Π)	33977.9 33593.4	381.8 H 384.0 H	1.0 1.1					C ↔ X, R	33973.7 33590.2	H H	(1)(4)
B (² Σ)	(27316)	(185.0) H	(0.5 ₃)					B → X, R	(27213)	H	(2)(5)(6)
X (² Σ)	0	390.5 H	1.5 ₅								
⁽⁶⁴⁾ Zn ¹³³ Cs ?		$(\mu = 43.165842_1)$ Diffuse V shaded absorption bands at 19363 and 19503 cm ⁻¹ .							JUL 1975		
									(1)		
⁽⁶⁴⁾ Zn ¹⁹ F		$(\mu = 14.6459379)$							JUL 1975		
D (² Σ)								D ← X, ^a R	(38633)	H	(1)
C (² Π)	(37359) (36987)	([596.8]) H ^Q ([601.5]) H ^Q						C ← X, ^a R	(37343.9) (36974.2)	H ^Q H ^Q	(1)
X (² Σ)	0	(628) H	(3.5)								

Zn₂: (1) W. Finkelburg, "Kontinuierliche Spektren", Springer (Berlin, 1938).

ZnBr: ^aFrom the analysis (8) of the absorption spectrum. An earlier analysis (3) of absorption measurements by (1) gave $\omega' \approx 250$, $\omega'' \approx 220$.

^bShading uncertain.

^cSuggested vibrational constants in (6).

(1) Walter, Barratt, PRS A 122, 201 (1929).

(2) Wieland, HPA 2, 46, 77 (1929).

(3) Howell, PRS A 182, 95 (1943).

(4) Wieland, in "Contribution à l'Etude de la Structure Moléculaire", Vol. comm. Victor Henri, Ed. Desoer, Liège (1948); p. 229.

(5) Ramasastry, Sreeramamurty, PNISI 16, 305 (1950).

(6) Patel, Rajan, IJP 42, 125 (1968).

(7) Rajan, Shah, IJPAP 7, 61 (1969).

(8) Gosavi, Greig, Young, Strausz, JCP 54, 983 (1971).

ZnCl: ^aNa D line chemiluminescence in Na/ZnCl₂ flames [(3), revised].

^b0-0 sequence only.

(1) See ref. (1) of ZnBr.

(2) See ref. (2) of ZnBr.

(3) Horn, Polanyi, Sattler, ZPC B 17, 220 (1932).

(4) Cornell, PR 54, 341 (1938).

(5) See ref. (4) of ZnBr.

(6) Patel, Rajan, IJPAP 5, 330 (1967).

ZnCs: (1) Barratt, TFS 25, 758 (1929).

ZnF: ^aDiffuse bands, predissociation.

(1) Rochester, Olsson, ZP 114, 495 (1939).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-4}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{64}\text{Zn}^1\text{H}$		$\mu = 0.99218372$ $D_0^0 = 0.851 \text{ eV}^a$								JUL 1975 A
C $^2\Sigma^+$	41090	1824	H 48	$[7.23]^b$		$[4.7]$	$[1.53_3]$	C \leftarrow X, V 41200	H	(6)
B $^2\Sigma^+$	27587.7	1020.7	Z 16.5	$[3.288]^c$		$[1.40]$	$[2.27_3]$	B \rightarrow X, R 27303.9	Z	(2)
A $^2\Pi_r$	23276.9 ^d	1910.2	Z 40.8	7.433_2^e	0.238 ₅	$[4.48_2]^f$	1.5119	A \rightarrow X, V 23431.8 ^g	Z	(1)(2)(3)(4)(5)(9)
X $^2\Sigma^+$	0	1607.6	Z 55.14 ^h	6.6794^i	0.2500 ^j	$[4.66]^k$	1.5949 ₀	ESR sp. ^l		
$(^{64})\text{Zn}^2\text{H}$		$(\mu = 1.95258556)$ $D_0^0 = 0.87_9 \text{ eV}^m$								JUL 1975 A
C $^2\Sigma^+$	(41110)	1313	H 24					C \leftarrow X, V 41204	H	(6)
A $^2\Pi_r$	n			$[3.736]^o$		$[1.3_1]^p$	$[1.520_2]$	A \rightarrow X, V 23391.5 ^g	Z	(3)(9)
X $^2\Sigma^+$	0	[1072]	H (28)	$[3.349_7]^q$		$[1.24_0]$	$[1.6054]$			
$(^{64})\text{Zn}^1\text{H}^+$		$D_0^0 = (2.5) \text{ eV}$								JUL 1975
A $^1\Sigma^+$	46700	1365	Z 15	5.767	0.105	4.0	1.716	A \rightarrow X, R 46431	Z	(1)(2)
X $^1\Sigma^+$	0	1916	Z 39 ^a	7.407	0.238	4.8	1.515			
$(^{64})\text{Zn}^2\text{H}^+$										JUL 1975
A $^1\Sigma^+$	46693.9	974.4	Z 7.6	2.928	0.042	1.0	1.717	A \rightarrow X, R 46501.7	Z	(3)
X $^1\Sigma^+$	0	1364.8	Z 19.8	3.766	0.107	1.0	1.514			

Zn^1H , Zn^2H :

^aShort extrapolation for the ground state.

^bAll lines diffuse; predissociation.

^cAll observed vibrational levels of $B^2\Sigma$ show perturbations by $A^2\Pi$ levels with $v \geq 1$. The rotational constants in (2) are satisfactorily reproduced by $B_v = 3.304 - 0.033(v + \frac{1}{2}) + 0.00060(v + \frac{1}{2})^2 - 0.00024_5(v + \frac{1}{2})^3$, except for $v=1, 2$, and 3 all of which are close to the intersection of the two potential curves.

^d $A_0 = + 342.66$, $A_1 = + 342.06$ [as recalculated in (9) from the data of (2)].

^eRotational constants for $v=0$ and 1 as recalculated in (9) from the data of (2). Λ -type doubling in $^2\Pi_{\frac{1}{2}}$, $\Delta v_{fe}(v=0) \approx + 0.26_9(J + \frac{1}{2}) - \dots$, and in $^2\Pi_{3/2}$ [see (3) and (2)].

^f $D_1 = 4.46 \times 10^{-4}$; $H_0 = + 1.3_4 \times 10^{-8}$, $H_1 = + 0.9 \times 10^{-8}$.

^g $J' = \frac{1}{2}$ (average of F_1 and $\{F_2\}$) relative to $N''=0$. A different definition was used in (2).

^h $w_e y_e = + 0.398$, $w_e z_e = - 0.4339$. Very rapid convergence. The constants [from (2)] lead to a discrepancy of nearly 6 cm^{-1} for the highest observed level, $v=5$.

ⁱSpin doubling, $\Delta v_{12}(v=0) = + 0.254(N + \frac{1}{2}) - \dots$ [(2), see also (7)], decreasing rapidly with increasing v .

j $- 0.03765(v + \frac{1}{2})^2 + 0.00897(v + \frac{1}{2})^3 - 0.001479(v + \frac{1}{2})^4$.

^k $D_1, \dots, D_5(10^{-4} \text{ cm}^{-1}) = 5.00, 5.49, 6.58, 8.40, 10.5$.

Also higher order terms, see (2).

^lIn Ar matrix at 4 K (8).

^mFrom the value for Zn^1H .

ⁿ $A_0 = + 342.82$, as recalculated in (9) from the data of (3).

^oRotational constants recalculated in (9) from data in (3). Λ -type doubling in $^2\Pi_{\frac{1}{2}}$, $\Delta v_{fe} \approx + 0.17_0(J + \frac{1}{2}) - \dots$, see (3).

Zn^1H , Zn^2H (continued):

$P_{H_0} = + 1.6 \times 10^{-8}$.

^qSpin doubling $\Delta v_{12} = + 0.131(N + \frac{1}{2})$, see (3).

(1) Watson, PR 36, 1134 (1930).

(2) G. Stenvinkel, Dissertation (Stockholm, 1936).
Ref. to earlier work are reviewed in this paper.

(3) Fujioka, Tanaka, Sci. Pap. IPCR (Tokyo) 32, 143 (1937).

(4) Stenvinkel, Svensson, Olsson, AMAF 26, No. 10, 1 (1939).

(5) Mrozowski, PR 58, 597 (1940).

(6) Khan, PPS 80, 599 (1962).

(7) Veseth, JP B 3, 1677 (1970).

(8) Knight, Weltner, JCP 55, 2061 (1971).

(9) Veseth, JMS 38, 228 (1971).

Zn^1H^+ , Zn^2H^+ :

^a $w_e y_e = - 0.2$.

(1) Bengtsson, Grundström, ZP 57, 1 (1929).

(2) Bengtsson-Knave, NARSSU Ser. IV, 8, No. 4 (1932).

(3) Gabel, Zumstein, PR 52, 726 (1937).

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{64})Zn^{127}I$		$(\mu = 42.512918_7)$								JUL 1975
E	44115	142	H 3					E → X, R	44073 H	(5)
D	(39911)	(80) ^a	H (1.3)					D → X, (39839) ^a	H	(7)
$C_2(^2\Pi)$	30125.8 ^b	248.2	H 0.72					$C_2 \leftrightarrow X,^c$	30138.2 ^b H	(2)(8)*
$C_1(^2\Sigma)$	29498.9	272.0	H 0.50	Bands in the region 16000 - 28600 cm ⁻¹ ; no analysis.				$C_1 \leftarrow X, V$	29523.2 H	(8)*
B ($^2\Sigma$)										
X ($^2\Sigma$)	0	223.4	H 0.6 ₃ ^d							
$(^{64})Zn^{(115)}In$		$(\mu = 41.075781_9)$								JUL 1975
		Two narrow emission continua near 22160 and 24370 cm ⁻¹ .								(1)
D ($^2\Sigma$)	c + 17732.0	107.0	H 1.0					D → C, ^a	V 17757.2 H	(1)
C ($^2\Sigma$)	c	56.1	H 0.1							
B ($^2\Pi$)	a + 18831.2	193.9 ^b	H 0.6							
A ($^2\Sigma$)	a + 18810.8	201.2	H 0.6					B → A, V	18854.8 H	(1)*
	a	146.7	H 0.7						18838.0 H	
$(^{64})Zn^{(39)}K ?$		$(\mu = 24.208838_9)$								JUL 1975
		V shaded diffuse absorption band at 24107 cm ⁻¹ .								(1)
$(^{64})Zn^{16}O$		$(\mu = 12.7939099_4)$ $D_0^0 \leq 2.8_2$ eV ^a								JUL 1975
		Unclassified, mostly R shaded emission bands in the region 17300 - 20500 cm ⁻¹ .								(4)
$(^{64})Zn^{(85)}Rb ?$		$(\mu = 36.470733_9)$								JUL 1975
		Unclassified absorption bands in the region 22500 - 24000 cm ⁻¹ .								(1)

ZnI: ^aOnly bands with $v'' \geq 15$ and $v' \leq 2$; neither the analysis nor the assignment to ZnI appear certain.

^bWieland (2) gives $T_e = 30117.6$, $v_{00} = 30129.5$.

^cAccording to (8) most of the diffuse emission bands of system D of (4) in the region $30500 - 31300 \text{ cm}^{-1}$ fit well into the C_2-X system.

^dAverage value from C_1-X and C_2-X .

- (1) Terenin, ZP 44, 713 (1927).
- (2) See ref. (2) of ZnBr.
- (3) Oeser, ZP 25, 699 (1935).
- (4) Rao, Rao, IJP 20, 49 (1946).
- (5) Ramasastry, IJP 22, 119 (1948)
- (6) See ref. (4) of ZnBr.
- (7) Ramasastry, IJP 23, 35 (1949).
- (8) See ref. (8) of ZnBr.

ZnIn: ^aSystem of complex appearance; more recently (2) attributed to $ZnIn_2$.

^b0-0 sequence only. It is assumed that $A(^2\Sigma)$ is the lower state.

- (1) Santaram, Winans, PR A 136, 57 (1964).
- (2) See ref. (1) of ZnTl.

ZnK, ZnRb:

- (1) See ref. (1) of ZnCs.

ZnO: ^aThermochemical value (mass-spectrom.)(1); (2)(3).

- (1) Anthrop, Searcy, JPC 68, 2335 (1964).
- (2) Hirschwald, Stolze, Stranski, ZPC (Frankfurt am Main) 42, 96 (1964).
- (3) See ref. (4) of ZnS.
- (4) Pešić, CCA 38, 313 (1966).

ZnRb: See ZnK.

State	T_e	w_e	$w_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{64}\text{Zn}^{(32)}\text{S})$		$(\mu = 21.3130477)$		$D_0^0 = 2.0_8 \text{ eV}^a$						JUL 1975
		The origin of two absorption continua with long wavelength limits at 35700 and 46500 cm^{-1} , formerly attributed to ZnS (1), appears doubtful; see (3)(4).								
$(^{64}\text{Zn}^{(80)}\text{Se})$		$(\mu = 35.517196_3)$		$D_0^0 = 1.3_7 \text{ eV}^a$						JUL 1975
$(^{64}\text{Zn}^{(130)}\text{Te})$		$(\mu = 42.844572_7)$		$D_0^0 = 0.9_5 \text{ eV}^a$						JUL 1975
		The origin of two absorption continua with long wavelength limits at 17830 and 31480 cm^{-1} , formerly attributed to ZnTe (1), appears doubtful; see (2).								
$(^{64}\text{Zn}^{(205)}\text{Tl})$		$(\mu = 48.730625_4)$								JUL 1975
		Emission continuum, $25400 - 26500 \text{ cm}^{-1}$.								(1)
		Broad, intense emission band at 21360 cm^{-1} , followed by weaker V shaded bands at 21440 , 21550 , 21660 , 21770 , 21880 cm^{-1} .								(1)
		Emission continuum, $17900 - 18700 \text{ cm}^{-1}$.								(1)
$(^{90}\text{Zr}^{(79)}\text{Br})$		$(\mu = 42.027022_4)$								JUL 1975
		Unclassified, mostly R shaded band heads in emission at $26600 - 26650$ and $26910 - 26980 \text{ cm}^{-1}$.								(1)*
System B:		Four 0-0 sequences ($w'-w'' \approx -3.5$) of narrow R shaded heads; in em.. Possibly quartet system.						$\left\{ \begin{array}{l} 26481.0 \text{ H} \\ 26305.2 \text{ H} \\ 26133.9 \text{ H} \\ 25959.6 \text{ H} \end{array} \right.$		(1)*
System C:		Four groups of narrow R shaded heads, three of the groups having the appearance of long 0-0 sequences ($w'-w'' \approx +6$); in emission. ⁴ $\Pi \rightarrow {}^4\Sigma$?						$\left\{ \begin{array}{l} 24396.0 \text{ H} \\ 24177.2 \text{ H} \\ 23936.3 \text{ H} \\ (23708) \end{array} \right.$		(1)*

ZnS: ^aThermochemical value (mass-spectrom.)(2)(3)(4).
(1) Sen Gupta, PRS A 143, 438 (1934).
(2) Colin, ICB 26, 1129 (1961).
(3) Marquart, Berkowitz, JCP 39, 283 (1963).
(4) De Maria, Goldfinger, Malaspina, Piacente, TFS 61,
2146 (1965).

ZnSe: ^aThermochemical value (mass-spectrom.)(1).
(1) See ref. (4) of ZnS.

ZnTe: ^aEstimated thermochemical value (2).
(1) Mathur, IJP 11, 177 (1937).
(2) See ref. (4) of ZnS.

ZnTe: (1) Santaram, Vaidyan, Winans, JP B 4, 133 (1971).

ZrBr: (1) Sivaji, Rao, PRIA A 70, 1 (1970).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e	r_e (Å)	Observed Transitions		References
								Design.	ν_{00}	
$(^{90}\text{Zr}^{35}\text{Cl})$		$(\mu = 25.1763829)$								JUL 1975
System A:		Three 0-0 sequences ($\omega' - \omega'' \approx +15$) of line-like heads. $\Omega' = \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \rightarrow {}^4\Sigma?$						R	35231.7 H 34816.4 H 34354.6 H	(1)*
System B:		Very complex system of R and V shaded band heads in the region 26300 - 27600 cm^{-1} ; in emission.							(26918)	(1)*
System C:		Four 0-0 sequences ($\omega' - \omega'' \approx +8$) of complex structure. ${}^4\Pi \rightarrow {}^4\Sigma?$						R	24704.6 H 24530.4 H 24343.8 H (24155)	(1)*
$(^{90}\text{Zr}^{19}\text{F})$		$(\mu = 15.6840882)$								JUL 1975
		The spectrum attributed to ZrF (1) was shown to be due to CuF (2).								
$(^{90}\text{Zr}^{127}\text{I})$		$(\mu = 52.623739_5)$								JUL 1975
		Groups of unclassified emission bands in the region 24800 - 26000 cm^{-1} .								(1)
System B:		Four 0-0 sequences ($\omega' - \omega'' \approx -2$) of line-like R shaded heads. Possibly quartet system.						R	25416.6 H 25276.6 H 25117.2 H 24958.6 H	(1)*
System C:		Four 0-0 sequences ($\omega' - \omega'' \approx +5$) of line-like band heads. ${}^4\Pi \rightarrow {}^4\Sigma?$						R	23564.8 H 23282.2 H 22995.4 H (22720)	(1)*
$^{90}\text{Zr}^{14}\text{N}$		$\mu = 12.1159579_3$		$D_0^0 = 5.8_1 \text{ eV}^a$						JUL 1975 A
A ${}^2\Pi_r$	b			[0.4798]			[1.702 ₉]	A \rightarrow X, c	17701.8 H 17133.0 H	(2)
X ${}^2\Sigma$	0			[0.4832]			[1.696 ₉]			

ZrCl₄: (1) Carroll, Daly, PRIA A 61, 101 (1961).

ZrF₄: (1) Afaf, PPS A 63, 544, 1156 (1950).
(2) Carroll, Daly, PPS A 70, 549 (1957).

ZrI₄: (1) Sivaji, Rao, PRIA A 70, 7 (1970)

ZrN: ^aThermochemical value (mass-spectrom.)(1).

^bA₀ ≈ + 567.

^cPerturbations.

(1) Gingerich, JCP 42, 14 (1968).

(2) J. K. Bates, T. M. Dunn (Dept. of Chemistry, U. of Michigan, Ann Arbor), abstract of paper Σ8 presented at the 27th Symposium on Molecular Structure and Spectra, Columbus, Ohio (1972).

State	T _e	w _e	w _e x _e	B _e	α _e	D _e (10 ⁻⁷ cm ⁻¹)	r _e (Å)	Observed Transitions		References
								Design.	ν ₀₀	
⁹⁰ Zr ¹⁶ O										AUG 1975 A
μ = 13.5790678 ₉ D ₀ ⁰ = 7.85 eV ^a I.P. = 6.1 eV ^b Additional unidentified systems in gas phase emission: a) Headless bands in the region 12600 - 13200 cm ⁻¹ ; no analysis. b) Isolated R shaded band (one R, one P branch) at 12203.1 cm ⁻¹ , accompanied by a weaker head at 12216.7 cm ⁻¹ . c) Mostly R shaded heads in the region 10500 - 11800 cm ⁻¹ ; ten- tative analysis (10) gives w _e ' = 862.9, w _e 'x _e ' = 8.8; w _e '' = 945.4, w _e ''x _e '' = 8.6; uncertain. and in matrix absorption at 17025 ^c and 19397 ^d cm ⁻¹ .										
f (3Δ)								f → a, R φ-system	33993.7 H 33888.4 H 33685.2 H	(7)(10)
e								e → (a), R δ-system	28780.3 ^e H ^Q 28620.1 ^e H ^Q 28501.7 ^e H ^Q	(7)(10)
E 1Σ ⁺	27212.4	843.2 ₇	Z 3.0 ₄	0.3951	0.0019	3.4	1.772 ₆	E ↔ X, ^{fg} R System A	27144.7 ₁ Z	(7)(10)(13)* (16)* (19) (21)(26)
D 1Δ	y + 19321.5	[835.4]	Z 2.5 ₆ H	0.3986	0.0021	3.8	1.764 ₈	D → A, R System B	19272.5 ₅ Z	(9)(14)* (16)* (21) (1)* (3)* (10)(11)* (16)* (17) (18)(20)(21) (32)
d 3Δ	x + 22314.9 x + 21894.3 x + 21594.3	820.6	H 3.3 ₁	[0.3953] [0.3926] [0.3896]	(0.0021)	[2.4] [1.8] [3.5]	1.776 ₁	d ↔ a, ^f R α-system	21631.48 Z 21548.46 Z 21536.36 Z	(1)* (12)* (16)* (21) (29)(32)
c 3Π _r	x + 18137.6 x + 18079.4 x + 18041.3	845.4	H ^R 3.6 ₄	[0.4058] ^h [0.4032] [0.3960]	(0.0023)	[3.9] [5.0] [2.4]	1.756	c ↔ a, ^f R β-system	17466.46 ⁱ Z 17745.89 ⁱ Z 17995.70 Z	(1)* (4) (11)* (16)* (17)(18)(21) (22)(23)* (27)(32)
b 3Φ _r	x + 16700.5 x + 16070.4 x + 15468.0	853.9	H ^R 3.1 ₄	[0.40438] [0.40368] [0.40307]	0.00191 ^j 0.00210 ^j 0.00198 ^j	[3.642] ^k [3.617] ^k [3.562] ^k	1.7514 ₃	b ↔ a, ^f R γ-system	16033.81 ^l Z 15741.31 ^l Z 15426.78 ^l Z	

ZrO: ^aThermochemical value (mass-spectrom.)(15)(24)(31)(34).
^bBy electron impact (30)(34).
^cIn a Ne matrix; $\Delta G'(\frac{1}{2}) = 872$. For tentative assignments of gas phase emission bands in the same region see (16).
^dIn a Ne matrix; $\Delta G'(\frac{1}{2}) = 836$.
^eThe stronger R heads are at 28512.0, 28630.4, and 28790.5 cm^{-1} .
^fAbsorption in stellar atmospheres (5)(8)(25).

ZrO (continued):

^gAbsorption in rare gas matrices (19).
^h Λ -type doubling, see (29).
ⁱ $v_{00}(^3\Pi_1 - ^3\Delta_1) = 18033.80$, $v_{00}(^3\Pi_2 - ^3\Delta_2) = 17804.1$.
^j $B_0 - B_1$; constants for $v=2$ in (27).
^k D_v values for $v=1, 2$ in (27).
^l $\{J'=0\}$ relative to $\{J''=0\}$. A different definition was used in (27).

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e (10^{-7}cm^{-1})	r_e (\AA)	Observed Transitions		References
								Design.	ν_{00}	
$^{90}\text{Zr}^{16}\text{O}$ (continued)										
B 1_{Π}	15443	859 ^m	3	[0.40154] ⁿ		[3.52]	[1.7583] ₂	B \leftrightarrow X, ^f g R	15383.41 ^o Z	(16)* (19) (28)*
A 1_{Δ}	y	938.1	H 1.8 ₀	[0.4167]	(0.0012)	[3.5]	[1.726] ₀			
a 3_{Δ_r}	x + 625.5 x + 287.9 ₁ ^p x	936.5	H ^R 3.4 ₇	[0.41573] [0.41475] [0.41328]	0.00173 ^j 0.00190 ^j 0.00178 ^j	[3.309] ^k [3.269] ^k [3.169] ^k	1.7285			
X 1_{Σ^+}	0	[969.7 ₆]	Z 4.9 ₀	[0.42263]	0.0023	[3.19]	1.7116	IR fundamental ^q		

ZrO (continued):

^mFrom the matrix (Ne) absorption spectrum, in good agreement with $\omega = 858$ from Kratzer's relation.

ⁿ Λ -type doubling, $\Delta v_{fe} = + 0.00024 \times J(J+1)$.

^o $\{J'=0\}$ relative to $J''=0$. A different definition was used in (28).

^pThe energy of a 3Δ above $X^1\Sigma$ is estimated (33) as $1700 \pm 250 \text{ cm}^{-1}$ from the temperature dependence of the integral absorption coefficients for the 0-0 bands of E-X and d-a. The triplet splittings derive from the observation (29) of two satellite bands of $\beta(0-0)$; see ⁱ.

^qIn a Ne matrix at 4 K (19).

- (1) Lowater, PPS 44, 51 (1932).
- (2) Meggers, Kiess, JRNBS 2, 309 (1932).
- (3) Lowater, PTRSL A 234, 355 (1935).
- (4) Tanaka, Horie, PPMSJ 23, 464 (1941).
- (5) Davis, ApJ 106, 28 (1947).
- (6) Kiess, PASP 60, 252 (1948).
- (7) Afaf, Nature 164, 752 (1949).
- (8) Herbig, ApJ 109, 109 (1949).
- (9) Afaf, PPS A 63, 674 (1950).
- (10) Afaf, PPS A 63, 1156 (1950).
- (11) Lagerqvist, Uhler, Barrow, AF 8, 281 (1954).
- (12) Uhler, AF 8, 295 (1954).
- (13) Uhler, Åkerlind, AF 10, 431 (1956).

ZrO (continued):

- (14) Åkerlind, AF 11, 395 (1956).
- (15) Chupka, Berkowitz, Inghram, JCP 26, 1207 (1957).
- (16) Gatterer, Junkes, Salpeter, Rosen, METOX (1957).
- (17) Ortenberg, SAAJ 5, 588 (1962).
- (18) Ortenberg, Glasko, SAAJ 6, 714 (1963).
- (19) Weltner, McLeod, Nature 206, 87 (1965); JPC 62, 3488 (1965).
- (20) Singh, Pathak, PPS 90, 543 (1967).
- (21) Nicholls, Tyte, PPS 91, 489 (1967).
- (22) Singh, Pathak, PPS 91, 497 (1967).
- (23) Schadee, Davis, ApJ 152, 169 (1968).
- (24) Brewer, Rosenblatt, AdHTC 2, 1 (1969).
- (25) Davis, Keenan, PASP 81, 230 (1969).
- (26) Liszt, Smith, JQSRT 11, 1043 (1971).
- (27) Tatum, Balfour, JMS 48, 292 (1973).
- (28) Balfour, Tatum, JMS 48, 313 (1973).
- (29) Lindgren, JMS 48, 322 (1973).
- (30) Rauh, Ackermann, JCP 60, 1396 (1974).
- (31) Ackermann, Rauh, JCP 60, 2266 (1974).
- (32) Schoonveld, Sundaram, ApJ 192, 207 (1974).
- (33) Veits, Gurvich, Kobylanskii, Smirnov, Suslov, JQSRT 14, 221 (1974).
- (34) Murad, Hildenbrand, JCP 63, 1133 (1975).

APPENDIX

Ag ₂	(10) Brown, Ginter, JMS <u>62</u> , 25 (1978).	Absorption spectrum.
AgBi	(4) Lochet, JP B <u>10</u> , 277 (1977).	Laser excited fluorescence.
AgCd, AgHg	(1) Kasai, McLeod, JPC <u>72</u> , 2324 (1975).	ESR sp. in rare gas matrices.
AgO	(5) Griffiths, Barrow, JP B <u>10</u> , 925 (1977). (6) Griffiths, Barrow, JCS FT II <u>73</u> , 943 (1977).	A ² Π → X ² Π. Electronic spectra in rare gas matrices.
AgZn	(1) Kasai, McLeod, JPC <u>72</u> , 2324 (1975).	See AgCd.
AlBr	(12) Ram, SpL <u>2</u> , 435 (1976). (13) Rosenwaks, JCP <u>65</u> , 3668 (1976).	a ³ Π → X ¹ Σ ⁺ in chemiluminescence. a ³ Π → X ¹ Σ ⁺ , b ³ Σ ⁺ → a ³ Π in chemiluminescence.
AlCl	(13) Rosenwaks, JCP <u>65</u> , 3668 (1976).	a ³ Π ← X ¹ Σ ⁺ , rotational analysis.
AlF	(30) Kopp, Lindgren, Malmberg, PS <u>14</u> , 170 (1976). (31) Rosenwaks, JCP <u>65</u> , 3668 (1976).	a ³ Π, A ¹ Π → X ¹ Σ ⁺ ; b ³ Σ ⁺ , c ³ Σ ⁺ → a ³ Π in chemiluminescence.
Al ¹ H, Al ² H	(29) Pelissier, Malrieu, JCP <u>67</u> , 5963 (1977).	Theoretical calculation of the ground and valence excited states.
AlI	(5) Rosenwaks, JCP <u>65</u> , 3668 (1976).	See AlBr.
AlO	(53) Frank, Krauss, ZN <u>31</u> a, 1193 (1976). (54) Lindsay, Gole, JCP <u>66</u> , 3886 (1977). (55) Sayers, Gole, JCP <u>67</u> , 5442 (1977).	D ₀ ⁰ = 5.17 eV. B ² Σ ⁺ → X ² Σ ⁺ in chemiluminescence. A ² Π _i → X ² Σ ⁺ in chemiluminescence.
Ar ₂	(25) Gillen, Saxon, Lorents, Ice, Olson, JCP <u>64</u> , 1925 (1976). (26) Saxon, Liu, JCP <u>64</u> , 3291 (1976). (27) Aziz, JCP <u>65</u> , 490 (1976). (28) Ng, Trevor, Mahan, Lee, JCP <u>66</u> , 446 (1977). (29) Aziz, Chen, JCP <u>67</u> , 5719 (1977).	³ Σ _u ⁺ well depth from scattering data, D _e = 0.78 eV, r _e = 2.33 Å. <u>Ab initio</u> calculations of ³ Σ _g ⁺ and ³ Σ _u ⁺ states. Ground state potential. Photoionization of Ar ₂ , I.P. = 14.54 eV. Ground state potential and molecular constants.
Ar ₂ ⁺	(6) Miller Ling, Saxon, Moseley, PR A <u>13</u> , 2171 (1976).	Photodissociation cross sections, 5650 - 6950 Å.

Ar ₂ ⁺ (cont'd)	(7) Moseley, Saxon, Huber, Cosby, Abouaf, Tadjeddine, JCP <u>67</u> , 1659 (1977). (8) Wadt, JCP <u>68</u> , 402 (1978).	Photofragment spectroscopy; $X^2\Sigma_u^+$, $^2\Sigma_g^+$, $^2\Pi_g$ potentials. $D_0^0 = 1.33$ eV. Calculated potential curves of low-lying states.
ArF, ArF ⁺	(3) Gardner, Karo, Wahl, JCP <u>65</u> , 1222 (1976).	Hartree-Fock potential energy curves for $X^2\Sigma^+$ and $^2\Pi$ states of ArF.
Ar ¹ H, Ar ² H	(3) Bassi, Dondi, Tommasini, Torello, Valbusa, PR A <u>13</u> , 584 (1976).	H-Ar potential from scattering data. $D_e^0 = 4.16$ meV, $r_e = 3.62$ Å.
ArKr	(4) Piper, Setser, Clyne, JCP <u>63</u> , 5018 (1975). (5) Bobetic, Barker, JCP <u>64</u> , 2367 (1976). (6) Nain, Aziz, MP <u>33</u> , 303 (1977). (7) Buontempo, Cunsolo, Dore, Maselli, JCP <u>66</u> , 1278 (1977). (8) Ng, Tiedemann, Mahan, Lee, JCP <u>66</u> , 5737 (1977).	Interaction of metastable Ar with Kr. Molecular emission at 7565 Å. Calculated ground state vibrational energy levels. Ar-Kr intermolecular potential. Translational absorption spectrum.
ArO	(5) Julianne, Krauss, Stevens, CPL <u>38</u> , 374 (1976).	Photoionization of ArKr, I.P. = 13.42 ₅ eV. Collision-induced oxygen $^1S_0 - ^1D_2$ emission near 5577 Å in argon. Calculated bound-bound spectrum.
ArO ⁺	(1) Ding, Karlau, Weise, CPL <u>45</u> , 92 (1977).	$^4\Sigma^-$ potential from O ⁺ -on-Ar scattering data; $D_e = 0.68$ eV, $r_e = 2.02$ Å.
ArXe	(3) See ref. (5) of ArKr. (4) Chashchina, Shreider, JAS <u>23</u> , 914 (1975). (5) Castex, JCP <u>66</u> , 3854 (1977). (6) See ref. (8) of ArKr.	Absorption spectra 1150-1500 Å. Potential curves. Photoionization of ArXe; I.P. = 11.98 ₅ eV.
AsF	(11) Vasudev, Jones, CJP <u>55</u> , 337 (1977).	Rotational analysis of two overlapping systems fO^+ , $eO^- \leftrightarrow X_21$ (previously called $B \leftrightarrow X$).
AsN	(7) Krishnamurty, Thomas, IJPAP <u>14</u> , 236 (1976).	Isotope shifts.
AsS	(6) Ashrafunnisa, Rao, Rao, IJP <u>49</u> , 580 (1975).	$A_1^+ - X_2$ Franck-Condon factors, potential functions.
AuCa	(2) Coquant, Houdart, CR B <u>284</u> , 171 (1977).	Rotational analysis of A-X, B-X; preliminary results.
AuLi	(2) Ihle, Langenscheidt, Zmbova, JCP <u>66</u> , 5105 (1977).	IR sp. in rare gas matrices; extrapol. gas phase frequencies $\Delta G(\frac{1}{2}) = 746$ and 705 cm ⁻¹ for Au ⁶ Li and Au ⁷ Li, respectively.

AuO	(2) Griffiths, Barrow, JCS FT II <u>23</u> , 943 (1977).	Absorption and emission spectra in rare gas matrices. Predicted gas phase constants $\nu_{00} \approx 25000$, $\omega' \approx 600$, $\omega'' \approx 675$.
AuSi	(6) Coquant, Houdart, CR B <u>284</u> , 171 (1977).	Rotational analysis of A-X ₁ , preliminary constants.
BaBr	(9) Hildenbrand, JCP <u>66</u> , 3526 (1977).	$D_0^0 = 3.71$ eV (mass-spectrometric value).
BaCl	(15) See ref. (9) of BaBr.	$D_0^0 = 4.48$ eV (mass-spectrometric value).
BaO	(41) Ackermann, Rauh, Thorn, JCP <u>65</u> , 1027 (1976). (42) Wormsbecher, Lane, Harris, JCP <u>66</u> , 2745 (1977). (43) Hocking, Pearson, Creswell, Winnewisser, JCP <u>68</u> , 1128 (1978).	I.P. = 6.85 eV (electron impact). Microwave optical double resonance, Stark effect; dipole moment of A $^1\Sigma^+$, $\mu_{el}(\nu=7) = 2.2_0$ D. Millimeter wave spectrum.
BaS	(6) Tiemann, Ryzlewicz, Törring, ZN <u>31</u> a, 128 (1976).	Rotation sp. of $^{138}\text{Ba}^{32}\text{S}$; $B_e = 0.10331430$, $\alpha_e = 0.00031509_5$, $\gamma_e = -4.47 \times 10^{-7}$, $D_e = 3.09_5 \times 10^{-8}$.
BeAr ⁺	(3) Subbaram, Coxon, Jones, CJP <u>54</u> , 1535 (1976).	A $^2\Pi_r \rightarrow X^2\Sigma^+$, high resolution analysis; molecular constants.
BeF	(17) Gohel, Shah, IJP <u>48</u> , 932 (1974).	A-X RKR Franck-Condon factors.
BeKr ⁺	(2) Coxon, Jones, Subbaram, CJP <u>55</u> , 254 (1977).	A $^2\Pi_r \rightarrow X^2\Sigma^+$, high resolution analysis.
B ¹ H	(24) Stern, Kaldor, JCP <u>64</u> , 2002 (1976). (25) Pyper, Gerratt, PRS A <u>355</u> , 407 (1977).	Many-body perturbation theory applied to eight states. Spin-coupled theory of molecular wavefunctions [$X^1\Sigma^+$].
Bi ₂	(12) Süzer, Lee, Shirley, JCP <u>65</u> , 412 (1976). (13) Teichman, Nixon, JCP <u>67</u> , 2470 (1977).	Photoelectron sp., I.P. = 7.53, 8.94 eV ($X^2\Pi_{ui}$) and 9.30 eV ($A^2\Sigma_g^+$). New electronic states of matrix-isolated Bi ₂ .
BiCl	(12) Kuijpers, Törring, Dymanus, CP <u>18</u> , 401 (1976).	Microwave sp.; constants for Bi ³⁵ Cl $B_e = 0.09212553$, $\alpha_e = 0.00040203$, ..., also hfs constants.
BiF	(16) Kuijpers, Dymanus, CP <u>24</u> , 97 (1977).	Microwave sp.; $B_e = 0.22998897$, $\alpha_e = 0.00150262$, ...; also hfs constants.
BO, BO ⁺ , BO ⁻	(23) Griffing, Simons, JCP <u>64</u> , 3610 (1976).	Theoretical study of BO ⁻ , I.P. = 2.79 eV.
Br ₂	(44) Le Roy, Macdonald, Burns, JCP <u>65</u> , 1485 (1976).	B and C state repulsive potential curves from a fit of calculated continuum absorption coefficients to experimental data; B-X and C-X transition moment functions.

- Br₂ (cont'd) (45) Zaraga, Nogar, Moore, JMS 63, 564 (1976).
- (46) Chang, Hwang, JMS 65, 430 (1977).
- (47) Chang, Hwang, JCP 67, 3624 (1977).
- (48) Tellinghuisen, CPL 42, 485 (1977).
- (49) Lindeman, Wiesenfeld, CPL 50, 364 (1977).
- (50) de Vlieger, Eisendrath, JP B 10, L463 (1977).
- BrCl (15) Wright, Spates, Davis, JCP 66, 1566 (1977).
- BrF, BrF⁺ (12) Clyne, Curran, Coxon, JMS 63, 43 (1976).
- (13) Clyne, McDermid, JCS FT II 73, 1094 (1977).
- BS (9) Bell, McLean, JMS 63, 521 (1976).
- C₂ (60) Tatarczyk, Fink, Becker, CPL 40, 126 (1976).
- (61) Cooper, Nicholls, SpL 2, 139 (1976).
- (62) Curtis, Engman, Erman, PS 13, 270 (1976).
- (63) Leach, Velghe, JQSRT 16, 861 (1976).
- (64) Bell, Branch, ApJ 212, 591 (1977).
- (65) Swamy, O'Dell, ApJ 216, 158 (1977).
- (66) Kini, Savadatti, JP B 10, 1139 (1977).
- (67) Chauville, Maillard, Mantz, JMS 68, 399 (1977).

B-X transition moment from absolute line absorption measurements. Estimated B state radiative lifetime 20 μ s; predissociation quantum yields near unity.

Resonance fluorescence with argon-ion laser excitation.

Resonance Raman study; fundamental and eight overtones investigated with high resolution.

Reassignment of the "E \rightarrow B" system to the transition D'(³ Π_g)_{2g} \rightarrow A'(³ Π_u)_{2u}. Vibrational constants.

Laser induced photodissociation; B \leftarrow X and C \leftarrow X relative absorptivities.

Hanle effect studies of several rotational levels of B(³ Π_u)_{0u}⁺, v'=40,45.

Laser-excited fluorescence from B ³ Π_0 ⁺; lifetime 18.5 μ s.

Laser excitation spectrum of BrF B ³ Π_0 ⁺ \leftarrow X ¹ Σ ⁺. Rotational analysis. Predissociation.

Laser-excited fluorescence from B ³ Π_0 ⁺; lifetime 24.7 μ s.

Two new emission systems, E ² Σ ⁺ \rightarrow X ² Σ ⁺ (v₀₀=47933.6) and E ² Σ ⁺ \rightarrow A ² Π_1 . Rotational and vibrational constants.

Lifetimes of single vibrational levels of d ³ Π_g ; τ =120 ns corresponding to f₀₀ \approx 0.025 for the Swan system.

Transition probability data for seven band systems.

High resolution lifetime studies of d ³ Π_g , C ¹ Π_g , D ¹ Σ_u ⁺, τ (v'=0)=123, 31.1, 18.1 ns, respectively. Corresponding oscillator strength for the Swan bands f₀₀=0.026₁.

Laser pyrolysis; rad. lifetime of d ³ Π_g (v=0) \approx 240 ns.

Phillips system; rot. dependence of Franck-Condon factors.

Franck-Condon factors for the Fox-Herzberg and Ballik-Ramsay bands.

Swan bands; relative intensities in discharge through CO.

Line positions and molecular constants for A ¹ Π_u -X ¹ Σ_g ⁺.

Rotational perturbations in A ¹ Π_u (v=1) by a previously unob-

C ₂ (cont'd)	(68) Langhoff, Sink, Pritchard, Kern, Strickler, Boyd, JCP <u>67</u> , 1051 (1977).	served level of c $^3\Sigma_u^+$ leading to revised constants for the c state ($T_e = 9227.4$, etc.). <u>Ab initio</u> study of perturbations between X $^1\Sigma_g^+$ and b $^3\Sigma_g^-$.
C ₂ ⁻	(13) Cederbaum, Domcke, Niessen, JP B <u>10</u> , 2963 (1977).	Theoretical calculation of I.P. = 3.60 eV.
Ca ₂	(5) Sakurai, Broida, JCP <u>65</u> , 1138 (1976). (6) Miller, Andrews, CPL <u>50</u> , 315 (1977); Miller, Ault, Andrews, JCP <u>67</u> , 2478 (1977).	Laser photoluminescence. Absorption and emission spectra in solid argon and krypton. Resolved vibrational structure 14000-16000 cm ⁻¹ , $\omega' \approx 111(\text{Ar})$, $117(\text{Kr})$; $\omega'' \approx 78(\text{Kr})$.
CaBr	(11) Puri, Mohan, IJPAP <u>14</u> , 512 (1976). (12) Hildenbrand, JCP <u>66</u> , 3526 (1977).	Extension of the C→X and D→X systems. $D_0^0 = 3.18$ eV (mass-spectrometric value).
CaCl	(15) Domaille, Steimle, Wong, Harris, JMS <u>65</u> , 354 (1977). (16) Domaille, Steimle, Harris, JMS <u>66</u> , 503 (1977). (17) Brinkmann, Telle, JP B <u>10</u> , 133 (1977).	B $^2\Sigma^+ - X^2\Sigma^+$, rotational analysis. See (16). X $^2\Sigma^+$ rotation spectrum using laser microwave optical double resonance. Rotational constants for X: $B_e'' = 0.152233$, $\alpha_e'' = 0.000800$, and B: $B_e' = 0.154700$, $\alpha_e' = 0.000889$. Spin-splitting constants $y_0'' = +0.00136$, $y_0' = -0.0652$. Ca*+HCl(or CCl ₂) chemiluminescence, A→X and B→X. $D_0^0 \geq 4.28$ eV.
Ca ¹ H	(25) Berg, Klynning, Martin, OC <u>17</u> , 320 (1976).	Laser excitation spectroscopy of the B $^2\Sigma - X^2\Sigma$ transition.
Ca ² H	(9) Kaving, Lindgren, PS <u>13</u> , 39 (1976).	Absorption spectrum 2800-3200 Å. Rotational analyses of the 5p complex (K $^2\Sigma$, L $^2\Pi$) and of the 4d complex (G $^2\Sigma$, J $^2\Pi$ only).
CaMg	(1) Miller, Ault, Andrews, JCP <u>67</u> , 2478 (1977).	Absorption in solid argon and krypton, vibrational structure 17300-19000 cm ⁻¹ .
CaO	(22) Andrews, Ault, JMS <u>68</u> , 114 (1977). (23) Benard, Slafer, Love, Lee, AO <u>16</u> , 2108 (1977). (24) Creswell, Hocking, Pearson, CPL <u>48</u> , 369 (1977). (25) Hocking, Pearson, Creswell, Winnewisser, JCP <u>68</u> , 1128 (1978).	IR spectra of matrix-isolated CaO; four isotopes. Modulated transmission spectroscopy of chemi-excited CaO. Absorption from a $^3\Pi$ and A' $^1\Pi$. Pure rotational spectrum, $B_e = 0.44445274$, $\alpha_e = 0.00331266$ for $^{40}\text{Ca}^{16}\text{O}$. See (25). Millimeter wave spectrum.

CaSr	(1) Miller, Ault, Andrews, JCP <u>67</u> , 2478 (1977).	Absorption in solid argon, vibr. structure 14400 - 15200 cm ⁻¹ .
Cd ₂	(6) Ault, Andrews, JMS <u>65</u> , 102 (1977).	UV absorption in solid argon and krypton, vibr. structure 35000 - 36700 cm ⁻¹ .
Cd ¹ H, Cd ² H	(11) Jourdan, Negre, Dufayard, Nedelec, JP(Paris) <u>37</u> , L-29 (1976). (12) Dufayard, Nedelec, JP(Paris) <u>38</u> , 449 (1977).	Lifetime of A ² Π, τ ≈ 70 ns.
CeI	(1) Chantry, JCP <u>65</u> , 4412 (1976). (2) Chantry, JCP <u>65</u> , 4421 (1976).	Lifetimes, Λ-doubling, hfs of A ² Π. Negative ion formation in CeI ₃ . D(Ce-I) ≥ 3.7 ₇ eV. Positive ions by electron impact on CeI ₃ . I.P.(CeI) = 5.9 eV.
CeO	(9) Ackermann, Rauh, Thorn, JCP <u>65</u> , 1027 (1976).	I.P. = 4.90 eV (electron impact).
C ¹ H	(50) Evenson, Radford, Moran, APL <u>18</u> , 426 (1971). (51) Carozza, Anderson, JOSA <u>67</u> , 118 (1977). (52) Levy, Hinze, ApJ <u>211</u> , 980 (1977). (53) Hammersley, Richards, ApJ <u>214</u> , 951 (1977).	Pure rotational transition by IR laser magnetic resonance. Radiative lifetime of A ² Δ, τ(v=0,1) = 511 ns. Predicted Λ-doubling spectrum of ¹³ CH. Ab initio calculation of the Λ-doubling in excited rotational levels of CH and CD.
C ² H	(9) See ref. (53) of C ¹ H.	
C ¹ H ⁺	(23) Erman, ApJ <u>213</u> , L89 (1977). (24) Elander, Oddershede, Beebe, ApJ <u>216</u> , 165 (1977).	f ₀₀ = 0.0072 for A-X, from improved lifetime measurements. Theoretical spectroscopic constants and lifetimes for A-X.
C ² H ⁺	(3) See ref. (24) of C ¹ H ⁺ .	
Cl ₂	(44) Wells, Zipf, JCP <u>66</u> , 5828 (1977). (45) Chang, Hwang, JCP <u>67</u> , 4777 (1977). (46) Hwang, Chang, JMS <u>69</u> , 11 (1978). (47) Coxon, Shanker, JMS <u>69</u> , 109 (1978).	Translational spectroscopy, dissociative excitation of Cl ₂ . Resonance Raman spectrum of gaseous chlorine, Δv ≤ 8. Resonance fluorescence of gaseous chlorine. Rotational analysis of B ³ Π ₀ + → X ¹ Σ ⁺ of ³⁵ Cl ₂ and ^{35,37} Cl ₂ in the chlorine afterglow emission spectrum. Constants for ³⁵ Cl ₂ : T _e = 17817.67, ω _e ' = 255.38, ω _e 'x _e ' = 4.59, ω _e 'y _e ' = -0.038, B _e ' = 0.16313, α _e ' = 0.00242, γ _e ' = -0.000057. Reinterpretation of the 0 _g ⁺ ← 0 _u ⁺ system observed by (13).
Cl ₂ ⁻	(8) Martinez de Pinillos, Weltner, JCP <u>65</u> , 4256 (1976). (9) Sullivan, Freiser, Beauchamp, CPL <u>48</u> , 294 (1977).	ESR sp. of Cl ₂ ⁻ in various ion pairs at 4 K. Gas phase photodissociation of Cl ₂ ⁻ ; broad peak at 3500 Å attributed to 2Σ _g ⁺ ← X 2Σ _u ⁺ .

- CAF, CAF⁺ (19) Fabricant, Muentner, JCP 66, 5274 (1977).
Molecular beam electric resonance; hf, Stark, Zeeman properties. $\mu_{el}(^+CAF^-) = +0.85$ D.
- CaO, CaO⁻ (18) Bulgin, Dyke, Jonathan, Morris, MP 32, 1487 (1976).
Photoelectron sp., I.P. = 10.87 eV, $\omega(CaO^+) \approx 1040$ in $X^3\Sigma^-$.
(19) Amano, Hirota, JMS 66, 185 (1977).
Microwave sp. in $X^2\Pi(v=1)$.
(20) Arnold, Whiting, Langhoff, JCP 66, 4459 (1977).
MCSCF+IC wavefunctions, properties of $X^2\Pi$, $A^2\Pi$.
(21) Langhoff, Dix, Arnold, Nicholls, Danylewych, JCP 67, 4306 (1977).
Theoretical intensity parameters for vibration-rotation bands.
(22) Mandelman, Nicholls, JQSRT 17, 483 (1977).
A-X band oscillator strengths, continuum absorption cross sections, electronic transition moment.
(23) Cooper, JQSRT 17, 543 (1977).
A-X electronic transition moment.
(24) Menzies, Margolis, Hinkley, Toth, AO 16, 523 (1977).
Fundamental vibration-rotation spectrum.
(25) Rigaud, Leroy, Le Bras, Poulet, Jourdain, Combourieu, CPL 46, 161 (1977).
A-X absorption cross sections.
(26) Wine, Ravishankara, Philen, Davis, Watson, CPL 50, 101 (1977).
A-X high resolution absorption cross sections.
- CN (74) Miller, Freund, Field, JCP 65, 3790 (1976).
Identification and characterization of a $4\Sigma^+$ by anticrossing spectroscopy.
(75) Bailey, ApJ 211, 596 (1977).
Abs. coefficients for the fundamental and first overtone vibration-rotation bands.
(76) Bacis, Cerny, d'Incan, Guelachvili, Roux, ApJ 214, 946 (1977).
 $A^2\Pi-X^2\Sigma$; absolute wavenumber measurements by Fourier spectrometry, analysis of the 0-0 band. Rotational constants.
(77) Dixon, Woods, JCP 67, 3956 (1977).
Laboratory microwave spectrum. Rotational and hfs constants for $X^2\Sigma^+(v=0,1)$.
- CN⁻ (3) Pacansky, Liu, JCP 66, 4818 (1977).
Hartree-Fock electron affinity of CN 3.29 eV.
- CO (163) Rao, in "Spectroscopy", International Review of Science, Physical Chemistry (2) 3 (ed. Ramsay), Butterworths, London (1976), p. 317.
Wavenumbers for the 1-0 and 2-0 vibr.-rot. bands of $^{12}C^{16}O$, CO laser lines. Improved Dunham coefficients.
(164) Fleming, JQSRT 16, 63 (1976).
Line strength and halfwidth measurements from far-infrared absorption spectra.

- CO (cont'd)
- (165) Bouanich, JQSRT 16, 1119 (1976).
 - (166) Ogilvie, Koo, JMS 61, 332 (1976).
 - (167) Todd, Clayton, Telfair, McCubbin, Pliva, JMS 62, 201 (1976).
 - (168) Chackerian, Valero, JMS 62, 338 (1976).
 - (169) Banna, Shirley, JESRP 8, 255 (1976).
 - (170) Hamnett, Stoll, Brion, JESRP 8, 367 (1976).
 - (171) Phillips, Lee, Judge, JCP 65, 3118 (1976).
 - (172) Chackerian, JCP 65, 4228 (1976).
 - (173) Corvilain-Berger, Verhaegen, CPL 50, 468 (1977).
 - (174) Domin, Domin, Rytel, APP A 51, 783 (1977).
 - (175) Huffaker, JMS 65, 1 (1977).
 - (176) Kirschner, Le Roy, Ogilvie, Tipping, JMS 65, 306 (1977).
 - (177) Kay, Van der Leeuw, Van der Wiel, JP B 10, 2513 (1977).
 - (178) Marcoux, Piper, Setser, JCP 66, 351 (1977).
 - (179) Ermler, Mulliken, Wahl, JCP 66, 3031 (1977).
 - (180) Phillips, Lee, Judge, JCP 66, 3688 (1977).
 - (181) Kirby-Docken, Liu, JCP 66, 4309 (1977).
 - (182) Hemminger, Cavanagh, Lisy, Klemperer, JCP 67, 4952 (1977).
 - (183) Provorov, Stoicheff, Wallace, JCP 67, 5393 (1977).
 - (184) Möhlmann, de Heer, CP 21, 119 (1977).

$X^1\Sigma$ dipole moment function and transition moments.
 Dunham potential energy coefficients.
 Infrared emission; precise line positions for the 1-0, 2-1, 2-0 transitions of $^{12}\text{C}^{16}\text{O}$. $\Delta v=1$ sequences measured up to $v'=20, 11, 4$ for $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, respectively. Dunham coefficients for all three molecules.
 Absolute intensities for the 4-0 vibr.-rot. band.
 Photoelectron spectrum at 132.3 eV.
 PE branching ratios, partial ionization cross sections.
 $d^3\Delta_1 \rightarrow X^1\Sigma$ fluorescence, $\tau(v'=3) = 4.7 \mu\text{s}$. Electronic transition moment variation, $(d-X)/(d-a)$ branching ratios.
 $X^1\Sigma^+$ dipole moment function.
 Theoretical $15(1s_0)$ and $26(1s_C)$ ionization potentials.
 Analysis of the 4th pos. system of $^{12}\text{C}^{16}\text{O}$ in the near UV.
 $X^1\Sigma^+$ RKR potential.
 Ground state dipole moment function.
 Energy loss spectra near the carbon K edge.
 IR radiative decay constants for the vibrational levels of $a^3\Pi$.
 Molecular orbital correlation diagrams.
 $A \rightarrow X$ fluorescence from photodissociation of CO_2 ; transition moment variation.
 Ground state dipole moment function (theor.).
 Stark effect in $d^3\Delta_1(v=4) \leftarrow a^3\Pi_r(v=0)$, $\mu_{el}(d^3\Delta, v=4) = 0.42 \text{ D } (^-\text{CO}^+)$.
 Laser excited fluorescence from $A^1\Pi$; lifetimes of unperturbed rotational levels $\sim 10.9 \text{ ns}$, longer for perturbed levels.
 Dependence on r of the electronic transition moment for the 3rd pos. gr. ($b \rightarrow a$).

- CO (cont'd) (185) Meerts, de Leeuw, Dymanus, CP 22, 319 (1977). Molecular beam electric resonance. Stark-Zeeman spectra in $v=0, J=1$ of $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$.
- (186) van Sprang, Möhlmann, de Heer, CP 24, 429 (1977). Radiative lifetimes of a $^3\Sigma^+(v=4\dots 9)$ 10.24...6.82 μs , b $^3\Sigma^+(v=0)$ 56 ns, c $^3\Pi(v=0)$ 16 ns, B $^1\Sigma^+(v=0)$ 34 ns, d $^3\Delta(v=1\dots 16)$ 7.30...2.94 μs
- (187) Norbeck, Merkel, Certain, MP 34, 589 (1977). Theor. dipole moment functions for a $^3\Pi$ and A $^1\Pi$.
- (188) Plummer, Gustafsson, Gudat, Eastman, PR A 15, 2339 (1977). Partial photoionization cross sections 18-50 eV.
- CO⁺, CO⁺⁺ (41) Janjic, Pesic, ApJ 209, 642 (1976). Rotational analysis of the 1st neg. system of $^{12}\text{C}^{18}\text{O}^+$.
- (42) Gagnaire, Goure, CJP 54, 2111 (1976). Rot. anal. of the CO⁺ A \rightarrow X 2-0 band; Λ doubling constants.
- (43) Möhlmann, de Heer, CPL 43, 170 (1976). Radiative lifetimes for A $^2\Pi_1(v=0\dots 9)$ 3.8₂...2.1₁ μs .
- (44) Carrington, Sarre, MP 33, 1495 (1977). A $^2\Pi \leftarrow$ X $^2\Sigma$ absorption in an ion beam.
- (45) See ref. (179) of CO.
- (46) Kay, Van der Leeuw, Van der Wiel, JP B 10, 2521 (1977). Auger decay of carbon-K ionized CO.
- (47) Lee, JP B 10, 3033 (1977). Cross sections for the production of B \rightarrow X fluorescence by photoionization.
- (48) Möhlmann, de Heer, CP 21, 119 (1977). Electronic transition moment function for the 1st negative system (B-X).
- CO⁻ (9) Zubek, Szmytkowski, JP B 10, L27 (1977). Comparison of experimental and calculated cross sections for resonant vibrational excitation of CO by electron scattering; derived ground state constants $\omega=1895\text{ cm}^{-1}$, $r_0=1.223\text{ \AA}$, I.P. = -1.52 eV, $\Gamma = 0.80\text{ eV}$.
- (10) King, McConkey, Read, JP B 10, L541 (1977). Negative-ion resonances associated with K-shell-excited states of CO.
- CP (8) Murthy, Gowda, Narasimhamurthy, Pramana 6, 25 (1976). B $^2\Sigma$ -A $^2\Pi$ RKR Franck-Condon factors.
- CrMo (1) Efremov, Samoilova, Gurvich, CPL 44, 108 (1976). Absorption spectrum near 4800 \AA .
- CS, CS⁺ (30) Coxon, Marcoux, Setser, CP 17, 403 (1976). A $^1\Pi \rightarrow$ X $^1\Sigma$, A $^2\Pi \rightarrow$ X $^2\Sigma$; intensity and wavelength measurements.
- (31) Domcke, Cederbaum, von Niessen, Kraemer, CPL 43, 258 (1976). Calculated He I photoelectron spectrum of CS.

CS, CS⁺ (cont'd)

- (32) Robbe, Schamps, JCP 65, 5420 (1976).
- (33) Black, Sharpless, Slanger, JCP 66, 2113 (1977).
- (34) Chong, Takahata, JESRP 10, 137 (1977).
- (35) Todd, JMS 66, 162 (1977).
- (36) Cossart, Horani, Rostas, JMS 67, 283 (1977).
- (37) Gauyacq, Horani, CJP, in press (1978).
- Cs₂, Cs₂⁺ (23) Benedict, Drummond, Schlie, JCP 66, 4600 (1977).
- (24) Klewer, Beerlage, Los, Van der Wiel, JP B 10, 2809 (1977).
- (25) Toader, Collins, Johnson, Mirza, PR A 16, 1490 (1977).
- (26) Gupta, Happer, Wagner, Wennmyr, JCP 68, 799 (1978).
- CsAr (5) Sayer, Ferray, Lozingot, Berlande, JP B 2, L293 (1976).
- CsBr, CsBr⁺ (22) Potts, Williams, JCS FT II 72, 1892 (1976).
- CsCl (23) See ref. (22) of CsBr, CsBr⁺.
- (24) Cederberg, JCP 66, 5247 (1977).
- CsHe (2) See ref. (5) of CsAr.
- CsI, CsI⁺ (20) See ref. (22) of CsBr, CsBr⁺.
- (21) Grossman, Hurst, Payne, Allman, CPL 50, 70 (1977).
- CsKr, CsNe (3) See ref. (5) of CsAr.
- CsXe (6) Marek, Niemax, PL A 57, 414 (1976).
- (7) Marek, JP B 10, L325 (1977).
- Ab initio calculation of CS valence states and perturbation parameters.
- CS(a³Π) produced in photodissociation of CS₂. Radiative lifetime τ(a³Π) ≈ 16 ms.
- Theoretical calculations of photoelectron spectra.
- High resolution measurement of the 2-0 vibr.-rot. band of ¹²C³²S and ¹²C³⁴S; improved vibr. and rot. constants.
- a³Π_r → X¹Σ⁺; rotational analysis, perturbations.
- A²Π_i → X²Σ⁺ of CS⁺; rotational analysis, perturbations.
- Absorption spectra 8000-13000 Å, interpreted as A¹Σ_u⁺ ← X¹Σ_g⁺ and b³Π_u ← X¹Σ_g⁺.
- Ion-pair formation in two-photon absorption of molecular cesium (5630-6350 Å).
- Molecular satellites of the 6²S-7²P doublet of cesium.
- Absorption studies in the visible and near visible region.
- Emission spectra of discharges in Cs-rare gas mixtures.
- He II photoelectron spectrum.
- Molecular beam electric resonance; hfs constants.
- Saturated photodissociation of CsI.
- Emission bands 3500-6400 Å.
- Time-resolved fluorescence.

- Cu₂ (14) Steele, JMS 61, 477 (1976).
 CuI (13) Nair, Tiemann, Hoefft, ZN 32 a, 1053 (1977).
 CuO (14) Appelblad, Lagerqvist, PS 13, 275 (1976).
 (15) Griffiths, Barrow, JCS FT II 73, 943 (1977).
 (16) Lefebvre, Pinchemel, Schamps, JMS 68, 81 (1977).
 (17) Pinchemel, Lefebvre, Schamps, JP B 10, 3215 (1977).
 CuS (6) Biron, CR B 283, 209 (1976).
 DyO (6) See ref. (9) of CeO.
 ErO (5) See ref. (9) of CeO.
 EuO (8) Dirscherl, Michel, CPL 43, 547 (1976).
 (9) See ref. (9) of CeO.
 (10) Murad, Hildenbrand, JCP 65, 3250 (1976).
 (11) Balducci, Gigli, Guido, JCP 67, 147 (1977).
 F₂ (21) Hay, Cartwright, CPL 41, 80 (1976).
 F₂⁺ (8) Banyard, Ellis, Tait, Dixon, JP B 7, 1411 (1974).
 (9) Guyon, Spohr, Chupka, Berkowitz, JCP 65, 1650 (1976).
 Fe¹H, Fe²H (6) McCormack, O'Connor, AA(Suppl.) 26, 373 (1976).
 (7) Wing, Cohen, Brault, ApJ 216, 659 (1977).
 GdO (9) See ref. (9) of CeO.
 (10) Yadav, Rai, Rai, CJP 54, 2429 (1976).
 Photoluminescence, lifetimes, and discharge excitation.
 On the hfs in the rotational spectrum.
 Rotational analyses of E²Δ→X²Π, H²Π→X²Π, I²Π→X²Π, P²Π→X²Π. Molecular constants, perturbations.
 Electronic spectra in rare gas matrices.
 Rotational analysis of a new system A²Σ⁺→X²Π₁. Upper state constants T₀=15531.90, ω_e=614.0, B₀=0.43828; large spin doubling.
 New ²Δ_{5/2}→X²Π_{3/2} transition. Upper state constants T₀=15317.24, B₀=0.42536.
 Rotational analysis of A→X 0-0 band.
 I.P. = 6.08 eV (electron impact).
 I.P. = 6.30 eV (electron impact).
 Dependence of reaction cross sections of Eu+O₂ on collisional energy; D₀⁰=4.97 eV.
 I.P. = 6.48 eV (electron impact).
 D₀⁰=4.85 eV (equilibrium mass-spectrometry).
 D₀⁰=4.84 eV (equilibrium mass-spectrometry).
 Rydberg, ionic, and valence interactions in the excited states of F₂.
 Ab initio studies of potential curves for low-lying states of F₂⁺ and F₂⁺⁺.
 Threshold photoelectron spectrum of F₂. Constants for X²Π_g, A=346, ω_e=1113, ω_ex_e=9.75.
 Wavelengths and line intensities for the 4920, 5320, and 8690 Å bands.
 Confirmation of the presence of FeH in sunspots and cool stars.
 I.P. = 5.75 eV (electron impact).
 Emission spectrum 19400-22500 cm⁻¹.

GeO

(27) Mummigatti, Jyoti, APH 42, 99 (1977).

$^1\text{H}_2$

(170) Dehmer, Chupka, JCP 65, 2243 (1976).

(171) Jette, JCP 65, 4325 (1976); 67, 2934 (1977) (erratum).

(172) Lee, Carlson, Judge, JQSRT 16, 873 (1976).

(173) Miller, Freund, JMS 63, 193 (1976).

(174) Wolniewicz, JMS 63, 537 (1976).

(175) Anderson, Watson, Sharpton, JOSA 67, 1641 (1977).

(176) Bunker, McLarnon, Moss, MP 33, 425 (1977).

(177) Glover, Weinhold, JCP 66, 303 (1977).

(178) Borrell, Guyon, Glass-Maujean, JCP 66, 818 (1977).

(179) Jungen, Atabek, JCP 66, 5584 (1977).

(180) Ford, Greenawalt, Browne, JCP 67, 983 (1977).

(181) Prochaska, Andrews, JCP 67, 1139 (1977).

(182) Bhattacharyya, Chiu, JCP 67, 5727 (1977).

(183) Kolos, Rychlewski, JMS 66, 428 (1977).

(184) Wolniewicz, Dressler, JMS 67, 416 (1977).

(185) Reddy, Varghese, Prasad, PR A 15, 975 (1977).

(186) Rumble, Sims, Purdy, JP B 10, 2553 (1977).

(187) Turner, Kirby-Docken, Dalgarno, ApJ(Suppl.) 35(3), 281 (1977).

(188) Vogler, Meierjohann, PRL 38, 57 (1977).

A-X RKR Franck-Condon factors.

High resolution measurement of relative photoabsorption and photoionization cross sections at 78 K, 715-805 Å.

Ab initio calculation of spin-rotation coupling in $c^3\Pi_u$.

Absolute absorption cross sections of H_2 and D_2 , 180-780 Å. Singlet-triplet anticrossings between $B^1\Sigma_u^+(3p\sigma)$ and $f^3\Sigma_u^+(4p\sigma)$.

Non-adiabatic corrections to the rotational energies of $X^1\Sigma_g^+(v=0\dots3)$.

Electron impact excitation of $G^1\Sigma_g^+$; lifetime ~ 30 ns.

Application of the effective vibration-rotation hamiltonian to H_2 and D_2 ; calculated vibration-rotation energies for H_2 ($v \leq 14$, $J \leq 5$).

Calculated potential curve for the $G,K^1\Sigma_g^+$ double minimum state.

Predissociation, 680-860 Å.

Rovibronic interactions in the absorption spectrum; an application of multichannel quantum defect methods.

Computation of nuclear motion and mass polarization adiabatic energy corrections for $X^1\Sigma_g^+$, $B^1\Sigma_u^+$, $C^1\Pi_u$, $D^1\Pi_u$.

Vibrational-rotational and pure rotational laser Raman spectrum in solid inert gas matrices at 12 K.

Theoretical radiative lifetime of $c^3\Pi_u(v=0) = 1.76$ ms.

Ab initio potential energy curves for $c^3\Pi_u$, $I^1\Pi_g$, $i^3\Pi_g$.

The E,F and $G,K^1\Sigma_g^+$ states of hydrogen. Adiabatic calculation of vibronic states.

Collision-induced fundamental IR absorption band.

Calculated oscillator strengths for the $C^1\Pi_u - X^1\Sigma_g^+$ Werner b..

Calculated electric quadrupole vibration-rotation transition probabilities for the ground state ($v \leq 14$, $J \leq 20$).

Predissociation of $c^3\Pi_u$.

- $^1\text{H}_2$ (cont'd) (189) Glass-Maujean, Breton, Guyon, PRL 40, 181 (1978). Accidental predissociation of $\text{D}^+ \cdot ^1\Pi_u^+(4p\pi)$.
 (190) Kligler, Rhodes, PRL 40, 309 (1978). Two-photon excitation of $\text{E,F } ^1\Sigma_g^+$.
 (191) Wicke, JCP 68, 337 (1978). G,K double-minimum state.
- $^1\text{H}^2\text{H}$ (52) Smirnov, Mazurenko, OS(Engl. Transl.) 41, 566 (1976). Calculation of the permanent dipole moment.
 (53) See ref. (174) of $^1\text{H}_2$.
 (54) Prasad, Reddy, JCP 66, 707 (1977). IR absorption; collision-induced fundamental band in HD + Kr and HD + Xe mixtures at room temperature.
 (55) Reddy, Prasad, JCP 66, 5259 (1977). IR absorption; collision-induced fundamental band of the pure gas.
 (56) Alemar-Rivera, Ford, JMS 67, 336 (1977). Non-adiabatic effects in the B, C, and E,F states of HD.
 (57) See ref. (184) of $^1\text{H}_2$.
 (58) See ref. (181) of $^1\text{H}_2$.
- $^2\text{H}_2$ (61) See ref. (174) of $^1\text{H}_2$.
 (62) See ref. (172) of $^1\text{H}_2$.
 (63) See ref. (178) of $^1\text{H}_2$.
 (64) See ref. (179) of $^1\text{H}_2$.
 (65) See ref. (180) of $^1\text{H}_2$.
 (66) See ref. (181) of $^1\text{H}_2$.
 (67) See ref. (184) of $^1\text{H}_2$.
- $^1\text{H}_2^+$ (28) van Asselt, Maas, Los, CP 5, 429 (1974). Laser-induced photodissociation of H_2^+ and D_2^+ in ion beams.
 (29) Colbourn, CPL 44, 374 (1976). The use of the electron reduced mass in the electronic Schrödinger equation for H_2^+ and its isotopes.
 (30) Ozenne, Durup, Odom, Pernot, Tabché-Fouhaillé, Tadjeddine, CP 16, 75 (1976). Laser photodissociation of H_2^+ , D_2^+ , HD^+ in ion beams. Comparison between experimental and ab initio computed fragment kinetic energy spectra.
 (31) Bishop, JCP 66, 3842 (1977). Relativistic corrections for H_2^+ and its isotopes.
 (32) Bishop, Cheung, PR A 16, 640 (1977). Calculated IR transition frequencies for H_2^+ , D_2^+ , HD^+ , HT^+ ,
 (33) Cohen, McEachran, Schlifer, CPL 49, 374 (1977). Hyperfine structure of H_2^+ . | DT^+ .
- $^1\text{H}^2\text{H}^+$, $^1\text{H}^3\text{H}^+$ (7) Colbourn, Bunker, JMS 63, 155 (1976). Accurate theoretical vibration-rotation energies and transition moments for HD^+ , HT^+ , DT^+ .
 (8) See ref. (30) of $^1\text{H}_2^+$.

$^1\text{H}^2\text{H}^+$, $^1\text{H}^3\text{H}^+$ (cont'd)

- (9) See ref. (31) of $^1\text{H}_2^+$.
(10) Thomas, Dale, Paulson, JCP 67, 793 (1977).
(11) See ref. (32) of $^1\text{H}_2^+$.
(12) Ray, Certain, PRL 38, 824 (1977).

$^2\text{H}_2^+$, $^2\text{H}^3\text{H}^+$, $^3\text{H}_2^+$

- (13) See ref. (28) of $^1\text{H}_2^+$.
(14) See ref. (7) of $^1\text{H}^2\text{H}^+$, $^1\text{H}^3\text{H}^+$.
(15) See ref. (30) of $^1\text{H}_2^+$.
(16) See ref. (32) of $^1\text{H}_2^+$.
(17) See ref. (10) of $^1\text{H}^2\text{H}^+$, $^1\text{H}^3\text{H}^+$.

$^1\text{H}_2^-$

- (7) Buckley, Bottcher, JP B 10, L635 (1977).

^1HBr

- (48) Johnson, Ramsey, JCP 67, 941 (1977).
(49) Niay, Bernage, Coquant, Fayt, CJP 55, 1829 (1977).

^2HBr

- (14) Bernage, Niay, JMS 63, 317 (1976).
(15) Fayt, Van Lerberghe, Guelachvili, Amiot, Bernage, Niay, MP 32, 955 (1976).
(16) See ref. (48) of ^1HBr .

^3HBr

- (4) Bernage, Niay, CJP 55, 1016 (1977).

$^1\text{HBr}^+$, $^2\text{HBr}^+$

- (8) Möhlmann, de Heer, CP 17, 147 (1976).

^1HCl

- (65) Guelachvili, OC 19, 150 (1976).

^2HCl

- (28) Niay, Coquant, Bernage, Bocquet, JMS 65, 388 (1977).

Photodissociation spectra of HD^+ and D_2^+ .

Calculated hyperfine structure in the IR spectrum of HD^+ .

Feshbach projection-operator calculation of the resonant states of H_2^- .

Molecular beam electric resonance, Stark hf structure.

Dunham potential coefficients.

High resolution measurements of the 5-0 IR band; Dunham coefficients.

1-0, 2-0, 3-0, 4-0 IR absorption bands of D^{79}Br and D^{81}Br .

Equilibrium constants; precise calculated wavenumbers for observed chemical laser lines.

Calculated equilibrium constants from the constants for HBr and DBr .

Radiative lifetimes of $\text{A } ^2\Sigma^+$, $\tau(v=0,1,2) = 4.5, 4.0, \text{ and } 3.6$ (DBr^+) μs .

Absolute wavenumber measurements of the 2-0 IR absorption band of H^{35}Cl and H^{37}Cl by Fourier spectrometry. Band origins and rotational constants.

IR 3-0 absorption band, high resolution measurements. Dunham coefficients. Extrapolated constants for ^3HCl .

- ${}^1\text{HCl}^+, {}^2\text{HCl}^+$ (6) Brown, Watson, JMS 65, 65 (1977).
 (7) Möhlmann, Bhutani, de Heer, CP 21, 127 (1977).
- ${}^1\text{HCl}^-$ (3) Gianturco, Thompson, JP B 10, L21 (1977).
 (4) Taylor, Goldstein, Segal, JP B 10, 2253 (1977).
 (5) Goldstein, Segal, Wetmore, JCP 68, 271 (1978).
- He_2 (68) Brutschy, Haberland, PRL 38, 686 (1977).
 (69) Dacre, CPL 50, 147 (1977).
 (70) Ermler, Mulliken, Wahl, JCP 66, 3031 (1977).
 (71) Orth, Ginter, JMS 64, 223 (1977).
 (72) Saxon, Gillen, Liu, PR A 15, 543 (1977).
 (73) Orth, Brown, Ginter, JMS 69, 53 (1978).
- $\text{He}_2^+, \text{He}_2^{++}$ (15) Blint, PR A 14, 2055 (1976).
 (16) Maas, Van Asselt, Nowak, Los, Peyerimhoff, Buenker, CP 17, 217 (1976).
 (17) See ref. (70) of He_2 .
 (18) Yagisawa, Sato, Watanabe, PR A 16, 1352 (1977).
- HeAr (7) Smith, Rulis, Scoles, Aziz, Nain, JCP 67, 152 (1977).
- He^1H (6) Toennies, Welz, Wolf, CPL 44, 5 (1976).
- Spin-orbit and spin-rotation coupling in doublet states; application to HCl^+ .
 Radiative lifetimes of $\text{HCl}^+ A {}^2\Sigma^+$, $\tau(v=0\dots 6) = 2.58 \dots 1.85 \mu\text{s}$.
 Dependence on r of the electronic transition moment.
- Theoretical evidence for short-lived resonances in electron scattering.
 Computation of resonant states of HCl^- .
 CI calculation on the resonant states of HCl^- .
- Crossed-atomic-beam study of the long-range parts of $A {}^1\Sigma_u^+$ and $C {}^1\Sigma_g^+$. The A state has a potential hump of 0.047 eV at 3.14 Å.
 Calculation of the He-He well depth (0.000908 eV at 3.03 Å).
 Molecular orbital correlation diagrams.
 $i {}^3\Pi_g \rightarrow a {}^3\Sigma_u^+$, $l {}^3\Pi_g \rightarrow a {}^3\Sigma_u^+$; constants for i, l . Perturbations.
Ab initio potential curves for ${}^1\Sigma_g^+$ states.
 Characterization of the ${}^1\Pi$ states associated with the UAO's 4p ... 9p. Wavenumber tables for transitions to $A {}^1\Sigma_u^+$ and molecular constants.
- Ab initio CI calculation of ${}^2\Sigma_g^+$, ${}^2\Sigma_u^+$, ${}^2\Pi_g$, ${}^2\Pi_u$ potential curves for He_2^+ .
Ab initio calculation of $X {}^2\Sigma_u^+$ and adjustment based on measurements of the rotational predissociation of ${}^4\text{He}_2^+$, ${}^3\text{He}_2^+$, ${}^3\text{He}^4\text{He}^+$.
- Accurate adiabatic potential curves for the ground state and eleven excited states of He_2^{++} .
- Crossed-beam differential scattering cross sections. Interatomic potential, $D_e = 0.0026_0$ eV, $r_e = 3.46$ Å.
- He-H potential from low-energy elastic scattering data; $D_e = 0.00046$ eV, $r_e = 3.72$ Å.

He ¹ H ⁺	(13) Stewart, Watson, Dalgarno, JCP <u>65</u> , 2104 (1976). (14) Price, MP <u>33</u> , 559 (1977).	Hartree-Fock calculation of excitation energies, oscillator strengths, etc.. Calculation of eigen-energies and widths of the quasi-bound states (orbiting resonances) of HeH ⁺ .
He ¹ H ⁺⁺	(3) Winter, Duncan, Lane, JP B <u>10</u> , 285 (1977).	Exact eigenvalues, electronic wavefunctions and their derivatives with respect to r for the lowest twenty states.
HeKr	(3) See ref. (7) of HeAr.	D _e = 0.0026 ₀ eV, r _e = 3.67 Å.
HeNe	(5) Grace, Johnson, Skofronick, JCP <u>67</u> , 2443 (1977).	Observation of orbiting resonances in He+Ne scattering.
HeXe	(4) See ref. (7) of HeAr.	D _e = 0.0024 ₁ eV, r _e = 3.95 Å.
¹ HF	(46) Guelachvili, OC <u>19</u> , 150 (1976). (47) Chan, Rao, ZN <u>32</u> a, 897 (1977). (48) Huffaker, JMS <u>65</u> , 1 (1977). (49) Pyper, Gerratt, PRS A <u>355</u> , 407 (1977).	Absolute wavenumber measurements of the 1-0 and 2-0 IR absorption bands by Fourier spectrometry. Dipole moment function. X ¹ Σ ⁺ RKR potential. Spin-coupled theory of molecular wave functions; application to HF (X ¹ Σ ⁺).
HfO	(10) Ackermann, Rauh, Thorn, JCP <u>65</u> , 1027 (1976).	First ionization potentials of the lanthanide monoxides.
Hg ₂	(14) Siara, Krause, PR A <u>11</u> , 1810 (1975). (15) Drullinger, Hessel, Smith, JCP <u>66</u> , 5656 (1977). (16) Smith, Drullinger, Hessel, Cooper, JCP <u>66</u> , 5667 (1977). (17) Komine, Byer, JCP <u>67</u> , 2536 (1977).	Formation and decay of Hg ₂ excimers in Hg-Ar mixtures. Experimental studies of mercury molecules. A theoretical analysis of mercury molecules.
HgAr	(11) Woodworth, JCP <u>66</u> , 754 (1977).	Optically pumped Hg ₂ studies. Electron-beam excited fluorescence from mixtures of Hg with high-pressure Xe, Kr, Ar.
HgBr	(14) Wilcomb, Bernstein, JMS <u>62</u> , 442 (1976). (15) Djeu, Mazza, CPL <u>46</u> , 172 (1977).	D ₀ ⁰ = 0.74 ₄ eV, from the Le Roy-Bernstein modified Birge-Sponer extrapolation for X ² Σ ⁺ . B→X in laser-excited fluorescence; τ = 23 ns.
HgCl	(14) See ref. (14) of HgBr.	D ₀ ⁰ = 1.06 ₆ eV.
HgCs	(6) Düren, JP B <u>10</u> , 3467 (1977).	Interpretation of experimental scattering cross sections with pseudopotential calculations.

- Hg¹H (16) Hehenberger, Laskowski, Brändas, JCP 65, 4559, 4571 (1976); Hehenberger, JCP 67, 1710 (1977). Weyl's theory applied to predissociation by rotation.
- HgI (17) See ref. (14) of HgBr. $D_0^0 = 0.387$ eV.
- HgK (6) See ref. (6) of HgCs.
- HgKr (1) See ref. (11) of HgAr.
- HgNa (5) See ref. (6) of HgCs.
- HgRb (3) See ref. (6) of HgCs.
- HgTl (3) Drummond, Schlie, JCP 65, 3454 (1976). Fluorescence spectra of bands in the blue and red regions. Potential of the Tl-Hg system as a laser.
- HgXe (1) Nikiforov, Plimak, Predtechenski, Shcherba, OS(Engl. Transl.) 41, 195 (1976). Formation of excited HgXe molecules.
(2) See ref. (11) of HgAr.
- ¹HI (33) Eland, Berkowitz, JCP 67, 5034 (1977). Photoionization mass-spectrometry. I.P. ($^2\Pi_{3/2}$) = 10.386 eV, I.P. ($^2\Pi_{1/2}$) = 11.049₅ eV.
(34) Ungemach, Schaefer, Liu, JMS 66, 99 (1977). $X^1\Sigma^+$, theoretical dipole moment function.
- ²HI (10) See ref. (33) of ¹HI. I.P. ($^2\Pi_{3/2}$) = 10.387 eV, I.P. ($^2\Pi_{1/2}$) = 11.0505 eV.
- HoO (6) See ref. (9) of CeO. I.P. = 6.17 eV (electron impact).
- I₂ (93) Glozman, Zakharenko, Melnikov, Tkachenko, Fofanov, OS(Engl. Transl.) 41, 519 (1976). Saturated absorption in I₂.
(94) Koo, Newton, Smith, Andrews, PL A 58, 449 (1976). Lifetimes of R(127) hf components in the B-X 11-5 band (~380 ns).
(95) Landsberg, CPL 43, 102 (1976). Nuclear hf splittings in the B-X system; no evidence for magnetic octupole coupling.
(96) Callear, Erman, Kurepa, CPL 44, 599 (1976). Lifetime of D $^1\Sigma_u^+$, $\tau = 15.5$ ns.
(97) Lehmann, SJQE 6, 442 (1976). Prediss. in B $^3\Pi_{0+u}$; dependence on rotation and vibration.
(98) Yee, JCS FT II 72, 2113 (1976). B $^3\Pi_{0+u} \leftrightarrow X^1\Sigma_g^+$ of $^{127}\text{I}_2$ and $^{129}\text{I}_2$. Rotational distortion constants. Identification and assignment of laser-excited molecular transitions.
- (99) Dalby, Petty-Sil, Pryce, Tai, CJP 55, 1033 (1977). Nonlinear resonant photoionization. New Rydberg 1_g state with $T_e = 53562.75$, $\omega_e = 241.41$, $B_e = (0.04029)$.

I₂ (cont'd) (100) Danyluk, King, CP 22, 59 (1977).

(101) Vigué, Broyer, Lehmann, JP B 10, L379 (1977).

(102) Williams, Fernández, Rousseau, CPL 47, 150 (1977).

(103) Tellinghuisen, CPL 49, 485 (1977).

IBr (25) Child, MP 32, 1495 (1976).

(26) Clyne, McDermid, JCS FT II 72, 2242 (1976).

(27) Tiemann, Dreyer, CP 23, 231 (1977).

(28) Wright, Havey, JCP 68, 864 (1978).

ICl (26) Clyne, McDermid, JCS FT II 72, 2242, 2252 (1976).

(27) Clyne, McDermid, JCS FT II 73, 1094 (1977).

IF (9) See ref. (26) of IBr and ICl.

(10) See ref. (27) of ICl.

InBr (7) Tiemann, Köhler, Hoeft, ZN 32 a, 6 (1977).

K₂, K₂⁺ (29) Herrmann, Leutwyler, Schumacher, Wöste, CPL 52, 418 (1977).

(30) Lemont, Giniger, Flynn, JCP 66, 4509 (1977).

KAr, KAr⁺ (11) Budenholzer, Gislason, Jorgensen, JCP 66, 4832 (1977).

KHe⁺
KKr⁺
KNe⁺ } (1) See ref. (11) of KAr, KAr⁺.

Two-photon sequential absorption spectroscopy. Constants for five excited electronic states ($T_e = 40389...42600 \text{ cm}^{-1}$). Fluorescence yield of individual hf components in the B state. A test of hyperfine predissociation.

B"¹ Π_{1u} repulsive potential function from resonance Raman scattering data.

Reassignment of the "H→B" system to the transition G→A'. Vibrational constants.

Predissociation and photodissociation of IBr. Potential curves for B and B'; new constants for B', $T_e = 17053$, $\omega_e = 123$, $\omega_e x_e = 4.4$, $B_e = 0.0323$.

B-X, spectroscopic constants, RKR potentials, Franck-Condon factors.

Ground state dipole moment $\mu_{el}(v=0) = 0.737 \text{ D}$.

B state lifetime $\tau(v=2,3,4) = 0.54 \text{ us}$.

See ref. (26) of IBr. B-X laser excitation spectrum, first observation of $v'=0$. New improved constants for B ³ Π_0^+ . B ³ Π_0^+ fluorescence decay lifetimes.

B-X excitation spectra; onset of predissociation in $v'=10$ at $J'=12$, leading to $D_0^0 \leq 2.8145 \text{ eV}$.

Hfs of $J=2 \leftarrow 1$ transition; new determination of the quadrupole coupling constants.

Two-photon ionization in a molecular beam.

B ¹ Π_{1u} radiative lifetime 12.2 ns.

Potassium ion-rare gas potentials from total cross-section measurements.

- Kr_2 , Kr_2^+ (15) Miller, Ling, Saxon, Moseley, PR A 13, 2171 (1976).
 (16) Ng, Trevor, Mahan, Lee, JCP 66, 446 (1977).
 (17) Wadt, JCP 68, 402 (1978).
- KrF , KrF^+ (13) Hay, Dunning, JCP 66, 1306 (1977).
 (14) Krauss, JCP 67, 1712 (1977).
 (15) Burnham, Searles, JCP 67, 5967 (1977).
- KrH^+ (4) Benoit, Kubach, Sidis, Pommier, Barat, JP B 10, 1661 (1977).
- KrO (3) Dunning, Hay, JCP 66, 3767 (1977).
- KrXe , KrXe^+ (7) Castex, JCP 66, 3854 (1977).
 (8) Ng, Tiedemann, Mahan, Lee, JCP 66, 5737 (1977).
 (9) Morlais, Rupin, Robin, CR B 284, 385 (1977).
- KXe^+ (1) See ref. (11) of KAr , KAr^+ .
- LaO (33) Ackermann, Rauh, Thorn, JCP 65, 1027 (1976).
 (34) Gole, Chalek, JCP 65, 4384 (1976).
 (35) Behere, Sardesai, Pramāṇa 8, 108 (1977).
- Li_2 , Li_2^+ , Li_2^- (36) Lam, Gallagher, Hessel, JCP 66, 3550 (1977).
 (37) Kusch, Hessel, JCP 67, 586 (1977).
 (38) Konowalow, Olson, JCP 67, 590 (1977).
 (39) Olson, Konowalow, CP 21, 393; 22, 29 (1977).
 (40) Pyper, Gerratt, PRS A 355, 407 (1977).
 (41) Wine, Melton, CPL 45, 509 (1977).
 (42) Watson, Cerjan, Guberman, Dalgarno, CPL 50, 181 (1977).
- Li^1H (23) Pyper, Gerratt, PRS A 355, 407 (1977).
- Photodissociation cross sections of Kr_2^+ , 5650-6950 Å.
 Photoionization in a molecular beam, I.P. = 12.87 eV.
 Calculated potential curves for low-lying states of Kr_2^+ .
Ab initio CI calculation of states dissociating to $\text{Kr} + \text{F}$, $\text{Kr}^+ + \text{F}^-$, $\text{Kr}(^3\text{P}) + \text{F}$.
 Theory, electronic structure.
 KrF B state radiative lifetime 9.0 ns.
 Charge-exchange processes in collisions between H^+ and Kr .
Ab initio CI calculation of low-lying electronic states.
 Absorption spectra in the far UV region.
 Photoionization study; I.P. = 11.757 eV.
- First ionization potentials of the lanthanide monoxides.
 Chemiluminescent spectra. $D_0^0 \geq 8.19$ eV.
 Potential energy curves.
- Intensity distribution in the A-X system.
 Analysis of $\text{A } ^1\Sigma_u^+ - \text{X } ^1\Sigma_g^+$. New constants.
 Theoretical vibrational energy levels for $\text{A } ^1\Sigma_u^+$.
 Calculated potential energy curves.
 Spin-coupled theory of molecular wavefunctions, application to Li_2 ($\text{X } ^1\Sigma_g^+$).
 $\text{A } ^1\Sigma_u^+$ radiative lifetime 18.0 ns.
 Calculated potential energy curves.
- Spin-coupled theory of molecular wavefunctions, application to LiH ($\text{X } ^1\Sigma^+$).

LiHe, LiHe ⁺	(10) Gatland, Morrison, Ellis, Thackston, McDaniel, Alexander, Viehland, Mason, JCP <u>66</u> , 5121 (1977).	Li ⁺ -He interaction potential.
LiK	(5) Zmbov, Wu, Ihle, JCP <u>67</u> , 4603 (1977).	Mass-spectrometric study, D ₀ ⁰ = 0.81 eV, I.P. = 4.69 eV.
LiNa, LiNa ⁺	(10) See ref. (5) of LiK.	D ₀ ⁰ = 0.90 eV, I.P. = 4.94 eV (constants for LiNa).
LuF	(4) Athénour, Féménias, Effantin, JP B <u>2</u> , 2893 (1976). (5) Effantin, Wannous, d'Incan, CJP <u>55</u> , 64 (1977). (6) Effantin, Bacis, d'Incan, PR A <u>15</u> , 1053 (1977).	Constants for X,A,B,E,F. Classification of bands belonging to eight systems in the region 3000 - 6500 Å. B ¹ Π → X ¹ Σ; hyperfine structure. I.P. = 6.79 eV (electron impact).
LuO	(11) See ref. (9) of CeO.	A-X discrete and continuous Franck-Condon factors.
Mg ₂	(12) Scheingraber, Vidal, JCP <u>66</u> , 3694 (1977). (13) Stevens, Krauss, JCP <u>67</u> , 1977 (1977). (14) Miller, Ault, Andrews, JCP <u>67</u> , 2478 (1977).	Electronic structure of the ground and excited states of Mg ₂ and Mg ₂ ⁺ . Absorption in solid argon and krypton, resolved vibrational structure 22300 - 23000 and 25000 - 28000 cm ⁻¹ .
Mg ₂ ⁺	(1) See ref. (13) of Mg ₂ .	Triplet-triplet transitions and intensities.
MgO	(28) Evans, Mackie, JMS <u>65</u> , 169 (1977). (29) Ikeda, Wong, Harris, Field, JMS <u>68</u> , 452 (1977).	Laser-induced photoluminescence spectra; B→X, B→A. Analysis of a ³ Π _i ∨ X ¹ Σ ⁺ perturbations.
MgSr	(1) Miller, Ault, Andrews, JCP <u>67</u> , 2478 (1977).	Absorption in solid argon and krypton; vibrational structure 16000 - 17100 cm ⁻¹ .
MnO	(14) Pinchemel, Schamps, CP <u>18</u> , 481 (1976). (15) Ferrante, Wilkerson, Graham, Weltner, JCP <u>67</u> , 5904 (1977).	Electronic structure. ESR sp. at 4 K; ⁶ Σ ⁺ ground state.
N ₂	(200) Becker, Engles, Tatarczyk, ZN <u>31</u> a, 673 (1976). (201) Dehmer, Dill, JCP <u>65</u> , 5327 (1976). (202) Hillier, Kendrick, JESRP <u>8</u> , 239 (1976). (203) Banna, Shirley, JESRP <u>8</u> , 255 (1976). (204) Kotlikov, OS(Engl. Transl.) <u>41</u> , 434 (1976). (204a) Hamnett, Stoll, Brion, JESRP <u>8</u> , 367 (1976).	C ³ Π _u ↔ B ³ Π _g (v" ≤ 13) K-shell spectrum of N ₂ . CI calc. of satellite peaks in core and valence PE spectra. Photoelectron spectrum at 132.3 eV. Hanle effect on a rotational level of B ³ Π _g . 50 eV. PE branching ratios, partial ionization cross sections 18 -

N_2 (cont'd) (205) Wells, Borst, Zipf, PR A 14, 695 (1976).

(206) Ermler, Mulliken, Wahl, JCP 66, 3031 (1977).

(207) Brennen, Shuman, JCP 66, 4248 (1977).

(208) Chutjian, Ajello, JCP 66, 4544 (1977).

(209) Hummer, Burns, JCP 67, 4062 (1977).

(210) Gürtler, Saile, Koch, CPL 48, 245 (1977).

(211) Rescigno, Langhoff, CPL 51, 65 (1977).

(212) Becker, Engels, Tatarczyk, CPL 51, 111 (1977).

(213) Plummer, Gustafsson, Gudat, Eastman, PR A 15, 2339 (1977).

(214) Rastogi, Lowndes, JP B 10, 495 (1977).

(215) Samson, Haddad, Gardner, JP B 10, 1749 (1977).

(216) Kay, Van der Leeuw, Van der Wiel, JP B 10, 2513 (1977).

(217) Woodruff, Marr, PRS A 358, 87 (1977).

(218) Yoshino, Tanaka, JMS 66, 219 (1977).

N_2^+ (75) Erman, PS 14, 51 (1976).

(76) Bouchoux, Goure, CJP 55, 1492 (1977).

(77) See ref. (206) of N_2 .

(78) Lee, JP B 10, 3033 (1977).

(79) Dick, Benesch, Crosswhite, Tilford, Gottscho, Field, JMS 62, 95 (1978).

N_2^{++} (7) Stockdale, JCP 66, 1792 (1977).

Translational spectroscopy of metastable fragments produced by dissociative excitation.

Molecular orbital correlation diagrams.

Spectrum of the Lewis-Rayleigh nitrogen afterglow.

Threshold photoelectron spectrum, 15.5 - 19.0 eV (800 - 650 Å).

Lifetimes of $x^1\Sigma_g^-$ (23.1 ns) and $y^1\Pi_g$ (19.9 ns).

High-resolution absorption spectrum, 990 - 440 Å. Rydberg-series leading to X, A, B, C of N_2^+ . Abs. cross sections.

K-shell photoionization.

C $^3\Pi_u$ radiative lifetimes, $\tau(v=0) = 36.6$ ns, $\tau(v=4) = 36.5$ ns.

Partial photoionization cross sections, 18 - 40 eV.

Collision-induced translational-rotational far-infrared absorption; quadrupole moment of N_2 , $|Q| = 1.21 \times 10^{-26}$ esucm². Total and partial photoionization cross sections from threshold to 100 Å.

Energy loss spectra and absolute oscillator strengths for shape resonances near the nitrogen K edge.

Photoelectron spectrum; partial cross sections as a function of energy from 16 to 40 eV.

High-resolution VUV absorption spectrum; homogeneous perturbation $c_4^1\Sigma_u^+(v=0) \sim b^1\Sigma_u^+(v=1)$.

Predissociation of C $^2\Sigma_u^+$; lifetimes $\tau(v=2) = 78.9$ ns, $\tau(v \geq 3) \approx 4$ to 5 ns.

B $^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$; perturbation B(v=1) \sim A(v=11).

Cross sections for the production of B \rightarrow X fluorescence by photoionization.

High-resolution study of B \rightarrow X bands.

High kinetic energy N^+ ions from decay of doubly ionized N_2 .

N_2^-	(11) King, McConkey, Read, JP B <u>10</u> , L541 (1977). (12) Veillette, Marchand, CJP <u>55</u> , 2134 (1977).	Negative-ion resonances associated with K-shell-excited states of N_2 . Negative ion resonances by electron impact in the 10.5-15.5 eV region.
Na_2	(41) Lam, Gallagher, Hessel, JCP <u>66</u> , 3550 (1977). (42) Woerdman, CPL <u>50</u> , 41 (1977). (43) See ref. (29) of K_2 , K_2^+ . (44) Woerdman, CPL <u>53</u> , 219 (1978).	Intensity distribution in the A-X system. Two-photon absorption. Experimental Franck-Condon factors for the A-X system from a comparative study of the saturation behaviour of Na_2 and Na transitions.
$NaAr$	(6) Smalley, Auerbach, Fitch, Levy, Wharton, JCP <u>66</u> , 3778 (1977). (7) Saxon, Olson, Liu, JCP <u>67</u> , 2692 (1977).	Analysis of the A-X fluorescence excitation spectrum; vibrational and rotational constants. $D_e^0 = 0.0048_2$ eV, $r_e(X^2\Sigma^+) = 4.991$ Å. Ab initio calculations for X $^2\Sigma$, A $^2\Pi$, B $^2\Sigma$.
NaI , NaI^+	(22) Anderson, Wilson, Ross, CPL <u>48</u> , 284 (1977).	Photodissociation in a molecular beam using linearly polarized light.
NaK	(9) Zmbov, Wu, Ihle, JCP <u>67</u> , 4603 (1977).	Mass-spectrometric study, $D_0^0 = 0.63$ eV, I.P. = 4.57 eV.
$NaNe$	(4) Ahmad-Bitar, Lapatovich, Pritchard, Renhorn, PRL <u>39</u> , 1657 (1977).	A-X laser excitation spectrum; spectroscopic constants. $D_e^0 = 0.0010_0$ eV, $r_e(X^2\Sigma^+) = 5.2_9$ Å.
NdO	(6) See ref. (9) of CeO.	I.P. = 4.97 eV (electron impact).
NeF	(2) Winter, Bender, Rescigno, JCP <u>67</u> , 3122 (1977).	Potential energy curves and predicted fluorescence.
$NeKr$, $NeKr^+$ $NeXe$, $NeXe^+$	(5) Castex, JCP <u>66</u> , 3854 (1977).	$NeXe$, absorption spectra in the far UV region.
N^1H	(56) Banerjee, Grein, JCP <u>66</u> , 1054, 2589 (1977). (57) Hsu, Smith, JCP <u>66</u> , 1835 (1977).	Calculated potential energy curves and spectroscopic constants for b $^1\Sigma^+$, d $^1\Sigma^+$. Lifetime of d $^1\Sigma^+(v=0)$ 46 ns (NH) and 62 ns (ND).
N^2H	(17) See ref. (57) of N^1H .	
Ni_2	(3) Moskovits, Hulse, JCP <u>66</u> , 3988 (1977). (4) Anderson, JCP <u>66</u> , 5108 (1977).	Matrix spectra in the visible and UV regions. Theory of UV spectra of Ni_2 .

- NO (210) Brzozowski, Erman, Lyyra, PS 14, 290 (1976).
 (211) Amiot, JP B 10, L317 (1977).
 (212) Sukumar, Bottcher, JP B 10, L335 (1977).
 (213) Freedman, CJP 55, 1387 (1977).
 (214) Goodman, Brus, JCP 67, 933 (1977).
 (215) Lee, JCP 67, 3998 (1977).
 (216) Möhlmann, de Heer, CPL 49, 588 (1977).
 (217) Patel, Kerl, Burkhardt, PRL 38, 1204 (1977).
 (218) Takezawa, JMS 66, 121 (1977).
 (219) Kristiansen, JMS 66, 177 (1977).
 (220) Dale, Johns, McKellar, Riggin, JMS 67, 440 (1977).
 (221) Amiot, Bacis, Guelachvili, CJP 56, 251 (1978).
 (222) Frueholz, Rianda, Kuppermann, JCP 68, 775 (1978).
- NO⁺, NO⁺⁺ (45) Shimauchi, SL 25, 1 (1976).
 (46) Natalis, Delwiche, Collin, Caprace, Praet, CPL 49, 177 (1977).
- O₂ (199) Galkin, OS(Engl. Transl.) 42, 486 (1977).
 (200) Guberman, JCP 67, 1125 (1977).
 (201) Goodman, Brus, JCP 67, 1482 (1977).
- Lifetimes for A,B,B',C,D,F. Predissociation rates and perturbations.
 Spectral coincidences between CO laser lines and absorption lines of NO.
 Interpretation of experimental results on preionization and predissociation via high-lying molecular states.
 C ²Π(v=0) ← X ²Π(v=0) two-photon absorption spectrum.
 The A ²Σ⁺(3s6) Rydberg state in solid rare gases.
 Energy loss spectrum.
 Radiative lifetimes (6.4₃ and 5.7₇ μs for v=1 and 2, resp.) and excitation energy (6.4 eV for v'=2) of b ⁴Σ⁻.
 Opto-acoustic high-resolution spectroscopy of the v=2←1 vibration-rotation transition.
 Rydberg series converging to b ³Π, A ¹Π, w ³Δ of NO⁺.
 On the determination of molecular parameters for NO (X ²Π).
 Term values for v=0.
 High-resolution laser magnetic resonance and infrared-radiofrequency double resonance spectroscopy of NO and its isotopes near 5.4 μm.
 IR study of the X ²Π v=0,1,2 levels of ¹⁴N¹⁶O. Preliminary results for v=0,1 of ¹⁴N¹⁷O, ¹⁴N¹⁸O, ¹⁵N¹⁶O.
 a ⁴Π←X²Π and b ⁴Σ⁻←X²Π by electron impact spectroscopy.
 Excitation energies of a ⁴Π(v=4) 5.22 eV and of b ⁴Σ⁻(v=0) 5.70 eV.
 NO⁺ A-X Franck-Condon factors.
 Ne I photoelectron sp. of NO; NO⁺ ground state levels observed to v=32.
 The b←X 0-1 band in the absorption spectrum of the earth's atmosphere.
 Accurate ab initio potential curve for X ³Σ_g⁻.
 Electronic spectroscopy and dynamics of the A, A', and c states in van der Waals solids.

- O_2 (cont'd) (202) Katayama, Ogawa, Ogawa, Tanaka, JCP 67, 2132 (1977).
 (203) Lee, JCP 67, 3998 (1977).
 (204) Saxon, Liu, JCP 67, 5432 (1977).
 (205) Lee, Slanger, Black, Sharpless, JCP 67, 5602 (1977).
- O_2^+ (53) Albritton, Schmeltekopf, Harrop, Zare, Czarny, JMS 67, 157 (1977).
 (54) Carrington, Roberts, Sarre, MP 34, 291 (1977).
 (55) Lambert, Goure, Albritton, CJP 55, 1842 (1977).
 (56) Samson, Gardner, JCP 67, 755 (1977).
 (57) Banna, Shirley, JESRP 8, 255 (1976).
- O^1H (127) Destombes, Marliere, Rohart, JMS 67, 93 (1977).
 (128) German, JCP 67, 5411 (1977).
 (129) Palmer, JCP 67, 5413 (1977).
- P_2 (28) Chong, Takahata, JESRP 10, 137 (1977).
 (29) Malicet, Brion, Daumont, CR C 284, 175 (1977).
 (30) Brion, Malicet, Daumont, CR C 284, 647 (1977).
 (31) Effantin, Bacis, Amiot, Verges, JMS 62, 79 (1978).
- P_2^- (1) Cederbaum, Domcke, Niessen, JP B 10, 2963 (1977).
- Pb_2 (8) Bondybey, English, JCP 67, 3405 (1977).
- VUV absorption spectra from $b^1\Sigma_g^+$ and $a^1\Delta_g$.
 Energy loss spectrum.
Ab initio CI study of the valence states.
 Quantum yields for the production of $O(^1D)$ by photodissociation of O_2 at 1160-1770 Å.
 Analysis of the $b^4\Sigma_g^- \rightarrow a^4\Pi_u$ 1st negative band system.
 Laser-induced predissociation spectrum of O_2^+ , $b \leftarrow a$. The b state predissociates via $b^4\Pi_g$.
 Comparison of experimental and theoretical line intensities in the $b \rightarrow a$ 0-0 band.
 Vibrational energy levels and dissociation energy of $X^2\Pi_g$.
 Photoelectron spectroscopy at 132.3 eV.
 Molecular constants for $X^2\Pi$ and $A^2\Sigma$ from the analysis of the Λ -doubling hfs, the pure rotational sp., and the $A-X$ 0-0 band.
 Predissociation and tunneling in the $A^2\Sigma^+$ state.
 Predissociation and tunneling in the $A^2\Sigma^+$ state.
 Theoretical calculations of photoelectron spectra.
 $b^3\Pi_g \rightarrow a^3\Sigma_u^+$; perturbations in $b(v=6,7)$ are attributed to a new $5\Sigma_g^+$ state.
 $A^1\Pi_g \rightarrow X^1\Sigma_g^+$, new data.
 High-resolution Fourier spectrometry of P_2 infrared emission. Analysis of a new system $A^1\Pi_g \rightarrow A'^1\Sigma_u^-$. Constants for A' : $T_e = 28521.79$, $\omega_e = 608.095$, $\omega_e x_e = 2.357$, $\omega_e y_e = 0.0016$, $B_e = 0.258731$, $\alpha_e = 0.001396$.
 Theoretical calculation of I.P. = 0.30 eV.
 Emission and laser excitation spectra in rare gas solids.
 Reassignment of gas phase data.

PCl	(3) Coxon, Wickramaaratchi, JMS <u>68</u> , 372 (1977).	Visible and near infrared emission excited in the reaction $\text{Ar}(^3\text{P}_{2,0}) + \text{PCl}_3$. Vibrational analyses of $\text{A } ^3\Pi \rightarrow \text{X } ^3\Sigma^-$ and $\text{b } ^1\Sigma^+ \rightarrow \text{X } ^3\Sigma^-$. Vibrational constants for all three states (P^{35}Cl and P^{37}Cl).
$\text{P}^1\text{H}, \text{P}^2\text{H}$	(16) Di Stefano, Lenzi, Margani, Xuan, JCP <u>68</u> , 959 (1978).	$\text{b} \rightarrow \text{X}$ observed in the VUV photolysis of PH_3 ; $T_0 = 14340 \text{ cm}^{-1}$.
PN, PN^+	(13) Atkins, Timms, SA A <u>33</u> , 853 (1977). (14) Bulgin, Dyke, Morris, JCS FT II <u>73</u> , 983 (1977). (15) Chong, Takahata, JESRP <u>10</u> , 137 (1977).	Matrix IR spectrum of PN. He I photoelectron spectrum; $\text{X } ^2\Sigma^+$, $\text{A } ^2\Pi$, $\text{B } ^2\Sigma^+$ of PN^+ . Theoretical calculations of photoelectron spectra.
PtAl ?	(1) Scullman, Cederbalk, JP B <u>10</u> , 3659 (1977).	Unclassified emission bands $16700 - 18300 \text{ cm}^{-1}$.
PtO	(6) Jansson, Scullman, JMS <u>61</u> , 299 (1976).	Optical absorption spectra in rare gas matrices.
$\text{Rb}_2, \text{Rb}_2^+$	(21) Gupta, Happer, Wagner, Wennmyr, JCP <u>68</u> , 799 (1978).	Absorption studies in the visible and near visible regions.
RhC	(7) Shadrin, Zhirnov, OS(Engl. Transl.) <u>38</u> , 367 (1975).	C-X Franck-Condon factors.
S_2	(52) Leone, Kosnik, APL <u>30</u> , 346 (1977).	Laser action on the B-X transition.
SbN	(3) Jenouvrier, Daumont, Pascat, CJP <u>56</u> , 30 (1978).	Electronic spectrum $3300 - 4000 \text{ \AA}$. Analysis of the $\text{A } ^1\Pi \rightarrow \text{X } ^1\Sigma^+$ system of four isotopes. Upper state strongly perturbed. Constants for $\text{X } ^1\Sigma^+$ of $^{121}\text{Sb}^{14}\text{N}$; $\omega_e = 864.80$, $\omega_e x_e = 4.75$, $B_e = 0.3988$, $\alpha_e = 0.0026$, $r_e = 1.8353$. The spectrum previously attributed to SbN is due to Sb_2 .
ScO	(23) Rao, Rao, Rao, Physica C <u>81</u> , 392 (1976).	A-X and B-X Franck-Condon factors.
SiC	(4) Graeffe, Juslén, Karras, JP B <u>10</u> , 3219 (1977).	Si $\text{K}\alpha$ X-ray emission spectrum from SiC.
SiO	(52) Chong, Takahata, JESRP <u>10</u> , 137 (1977).	Theoretical calculations of photoelectron spectra.
SiS	(16) Atkins, Timms, SA A <u>33</u> , 853 (1977).	Matrix IR spectrum.
Sn_2	(3) Teichman, Epting, Nixon, JCP <u>68</u> , 336 (1978).	Raman sp. in solid argon; $\omega_e \approx 188$, $\omega_e x_e \approx 0.53$.
Sr_2	(1) Miller, Ault, Andrews, JCP <u>67</u> , 2478 (1977).	Absorption in solid argon and krypton, vibrational structure from 13400 to 14600 cm^{-1} .

SrO	(36) Hocking, Pearson, Creswell, Winnewisser, JCP <u>68</u> , 1128 (1978).	Millimeter wave spectrum.
TaO	(8) See ref. (9) of CeO.	I.P. = 7.92 eV (electron impact).
TbO	(6) See ref. (9) of CeO.	I.P. = 5.62 eV (electron impact).
TiO	(64) Kovács, El Agrab, APH <u>42</u> , 67 (1977). (65) Steele, Linton, JMS <u>62</u> , 66 (1978).	On the anomalous triplet splitting of C $^3\Delta_r$. Flame spectroscopy; C-X radiative lifetimes and oscillator strengths, $\tau = 37, 29, 28$ ns for $v'=0, 1, 2$, respectively.
TmO	(6) See ref. (9) of CeO.	I.P. = 6.44 eV (electron impact).
U ₂	(1) Gorokhov, Emel'yanov, Khodeev, HT(USSR) <u>12</u> , 1156 (1974).	Mass-spectroscopic investigation; $D_0^0 = 2.25$ eV.
UN	(2) Green, Reedy, JCP <u>65</u> , 2921 (1976).	Identification in argon matrices.
V ₂	(2) Ford, Huber, Klotzbücher, Kündig, Moskovits, Ozin, JCP <u>66</u> , 524 (1977).	Matrix study.
Xe ₂ ⁺	(7) Wadt, JCP <u>68</u> , 402 (1978).	Calculated potential curves for low-lying states.
XeF	(18) Smith, Kobrinsky, JMS <u>62</u> , 1 (1978).	$B \leftarrow X$; $T_e = 28813.9$, $\omega'_e = 308.2$, $\omega'_e x'_e = 1.43$, $\omega''_e = 225.1$, $\omega''_e x''_e = 10.6$.
YbCl	(3) Lee, Zare, JMS <u>64</u> , 233 (1977).	Chemiluminescent spectrum, $A_1, A_2, B \rightarrow X$. Vibrational const..
YbF	(4) See ref. (3) of YbCl.	Vibr. constants for $A_2 \rightarrow X$; A_1 and B strongly perturbed.
Yb ¹ H, Yb ² H	(8) Van Zee, Seely, Weltner, JCP <u>67</u> , 861 (1977).	ESR and optical spectroscopy in argon matrices at 4 K.
YbO	(6) See ref. (9) of CeO.	I.P. = 6.55 eV (electron impact).
YF, YF ⁺	(8) Shenyavskaya, Gurvich, JMS <u>68</u> , 41 (1977).	Rotational analysis of $b^3\phi \rightarrow a^3\Delta$ of YF. New rotational constants.
Y ¹ H, Y ² H	(1) Bernard, Bacis, CJP <u>55</u> , 1322 (1977).	Analysis of singlet and triplet systems of YH and YD.
YO	(21) Chalek, Gole, JCP <u>65</u> , 2845 (1976).	Chemiluminescence spectrum. Analysis of $A'^2\Delta \rightarrow X^2\Sigma^+$; $T_e = \begin{cases} 14870.4 \\ 14531.2 \end{cases}$ $\omega'_e = \begin{cases} 794.9 \\ 794.0 \end{cases}$, $\omega''_e = 862.0$.
Zn ₂	(2) Hay, Dunning, Raffanetti, JCP <u>65</u> , 2679 (1976).	<u>Ab initio</u> calculation of electronic states dissociating to $^1S + ^1S, ^3P, ^1P$.

- Zn₂ (cont'd) (3) Ault, Andrews, JMS 65, 102 (1977).
- Zn¹H, Zn²H (10) Dufayard, Nedelec, JP(Paris) 38, 449 (1977).
- ZrN (3) Kabankova, Moskvitina, Kuzyakov, VMUK 16(5), 620 (1975). For engl. transl. see MUCB 30(5), 80 (1975).
- (4) Bates, Dunn, CJP 54, 1216 (1976).
- ZrO (35) Phillips, Davis, ApJ 206, 632 (1976).
- (36) Phillips, Davis, ApJ(Suppl.) 32(3), 537 (1976).
- (37) Lauchlan, Brom, Broida, JCP 65, 2672 (1976).

UV absorption in solid argon and krypton; vibrational structure 38300-40000 cm⁻¹.

Lifetimes (≈ 75 ns), Λ -doubling, hfs in A ² Π .

Electronic absorption spectrum.

The yellow and violet emission systems.

A new ¹ $\Sigma \rightarrow ^1\Sigma$ system of ZrO; $\nu_{00} = 17050.47$, $B'_0 = 0.40479$ [observed in matrix absorption (19) at 17025 cm⁻¹, see ^c on p. 687].

B \rightarrow X system; 18 additional bands, improved upper and lower state constants.

Laser photoluminescence in neon at 4 K. Tentative identification of two new infrared transitions, B \rightarrow A and b' ³ $\Pi \rightarrow$ a ³ Δ .

